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Full-f/Total-f XGC1: Present Status and Future Plans

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On behalf of

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SciDAC-3 Center for Edge Physics Simulation (EPSi)

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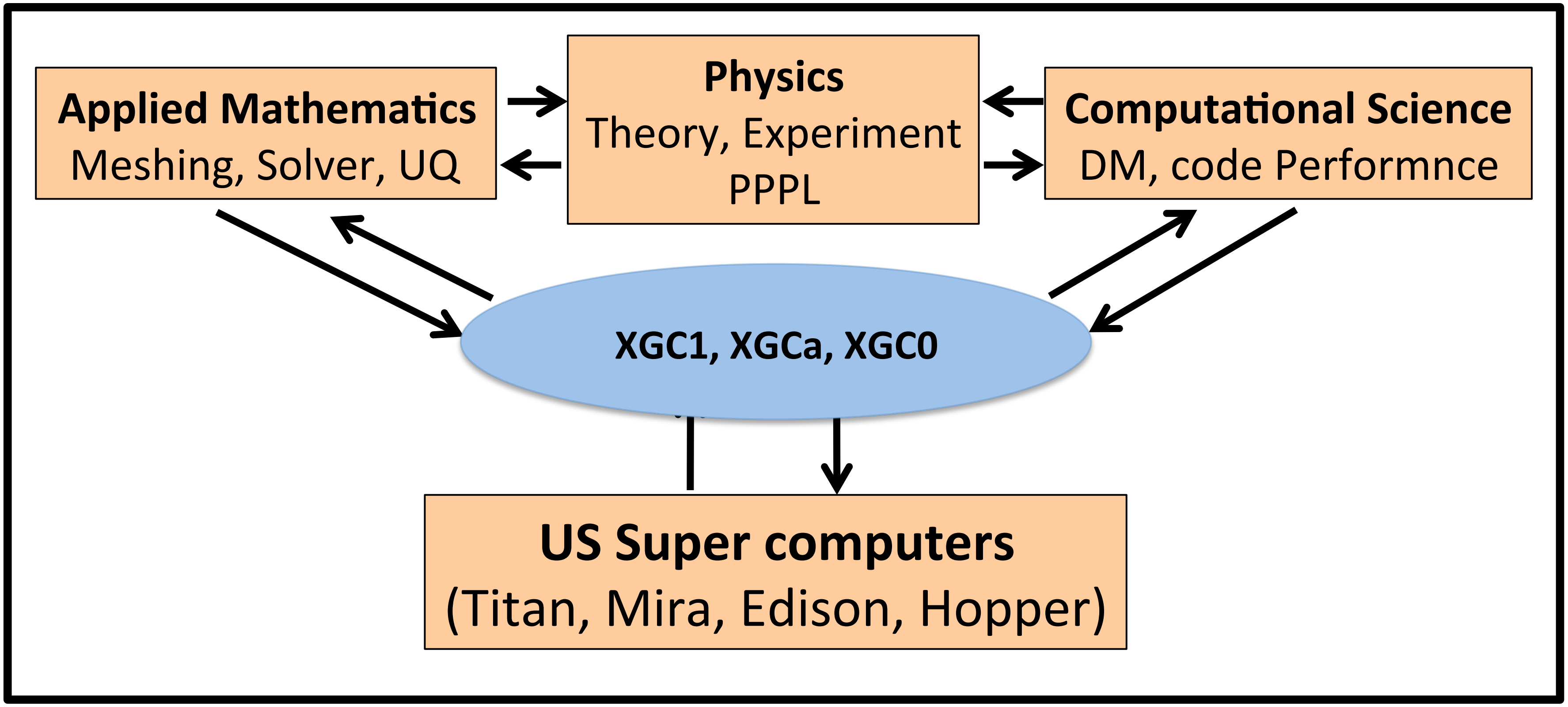
PRINCETON PLASMA PHYSICS LABORATORY

Edge Physics Simulation

Outline

1) Brief introduction to XGC family codes
2) Present Capability of XGC1
   - Kinetic ion physics with MC neutral particles
   - New physics with kinetic electrons
   - Starting the quest for the L-H transition physics
3) Future Plans for XGC1 (Brief)
   - Impurity physics
   - L-H transition physics
   - E&M
   - Multiscale time integration between XGC1 and XGCa
   - 3D RMP penetration and transport
4) Summary

The XGC Program is built on multi-disciplenary collaboration among physicists, applied mathematicians and computational scientists



Full-f Gyrokineic code XGC1 in diverted geometry

XGC1: X-point included Gyrokinetic Code 1

- **To build a gyrokinetic numerical tokamak-edge**
  - Heat and torque (and particle) input profiles in the core
  - Edge plasma self-organizes with core plasma, in the absence of an artificial core-edge boundary
- **Edge plasma is in a non-thermal equilibrium state and requires a non-perturbative kinetic simulation**
  - In contact with material wall with neutral recycling, radiative loss, wall-sheath
  - Non-Maxwellian, requiring nonlinear collisions
  - Magnetic separatrix geometry: Orbit loss and X-transport
  - Steep pedestal, with the gradient-width being ~ ion banana width
  - Blobs: $\delta n/n = \mathcal{O}(1)$
- **Nonlocal self-organization among overlapping multi-scale physics**
  - Neoclassical, turbulence, neutral particles with atomics physics, and wall

→XGC1 is designed to study such plasmas

-- Requires **extreme scale computing (2014 award ~300M hrs)**

XGC family codes: XGC1, XGCa and XGC0

All three codes push particles in 3D x-space + 2D in v-space

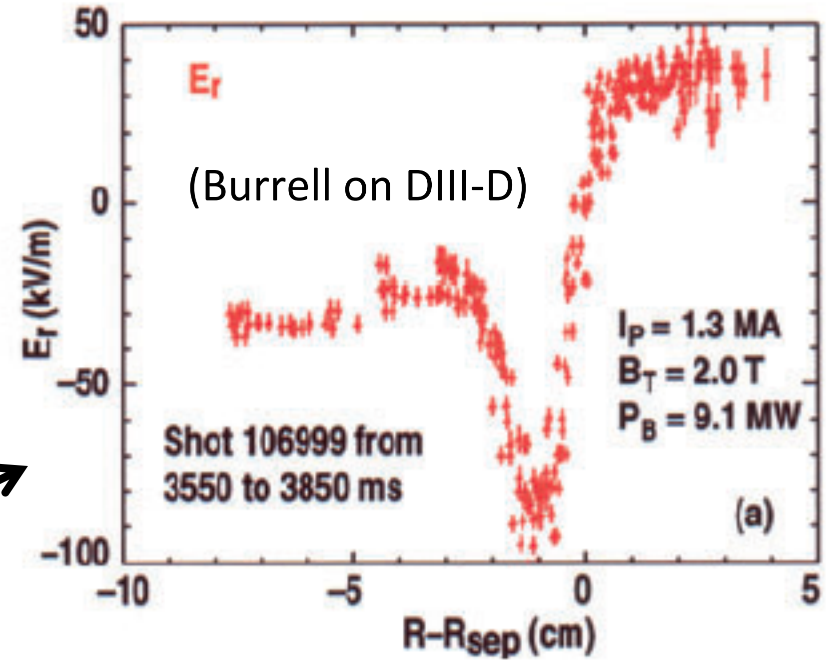
- In realistic diverted geometry
- Monte Carlo neutral atoms with CX and ionization interactions with plasma
- Uses logical sheath at limiter wall

- **XGCa: Gyrokinetic neoclassical version**
  - Axysymmetric electrostatic-potential solver version of XGC1
  - Solves not only for E_r, but also for E_θ
  - Automatically includes the gyroviscosity and the gyroviscous cancellation, as in XGC1
  - Nonlinear Fokker-Planck-Landau collision
  - ~10-100X faster than XGC1
  - Impurity particles, raditive loss and anomalous transport are to be added

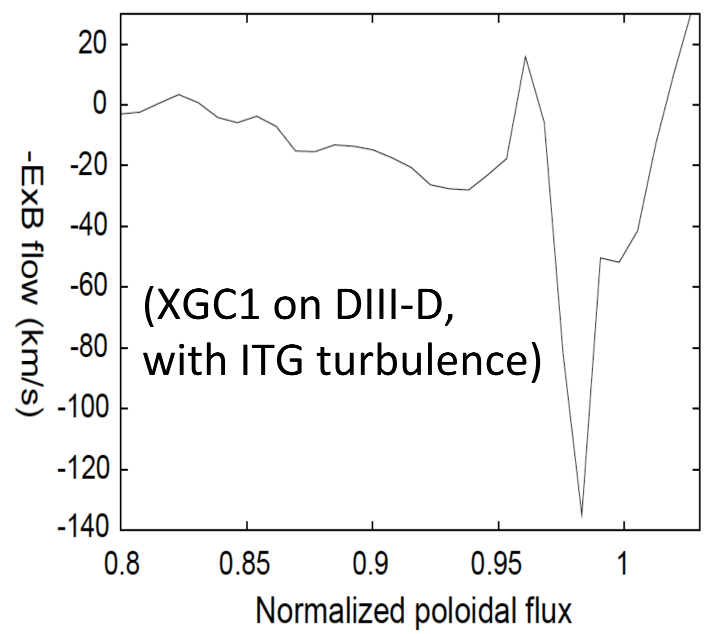
- **XGC0: Drift-kinetic neoclassical version**
  - Flux-surface averaged potential solver
  - Has more complete impurity particle routines, including radiative loss
  - Conservative linear Monte Carlo collision [Boozer, Wang, Lin …]
  - Uses anomalous transport and viscosity models

XGC family codes produce all-scale observables from particle Eq. motion and Poisson-Ampere eqs.

In H-mode experiment, a sharp negative E_r-well forms just inside separatrix



→ XGC1 reproduces this phenomenon



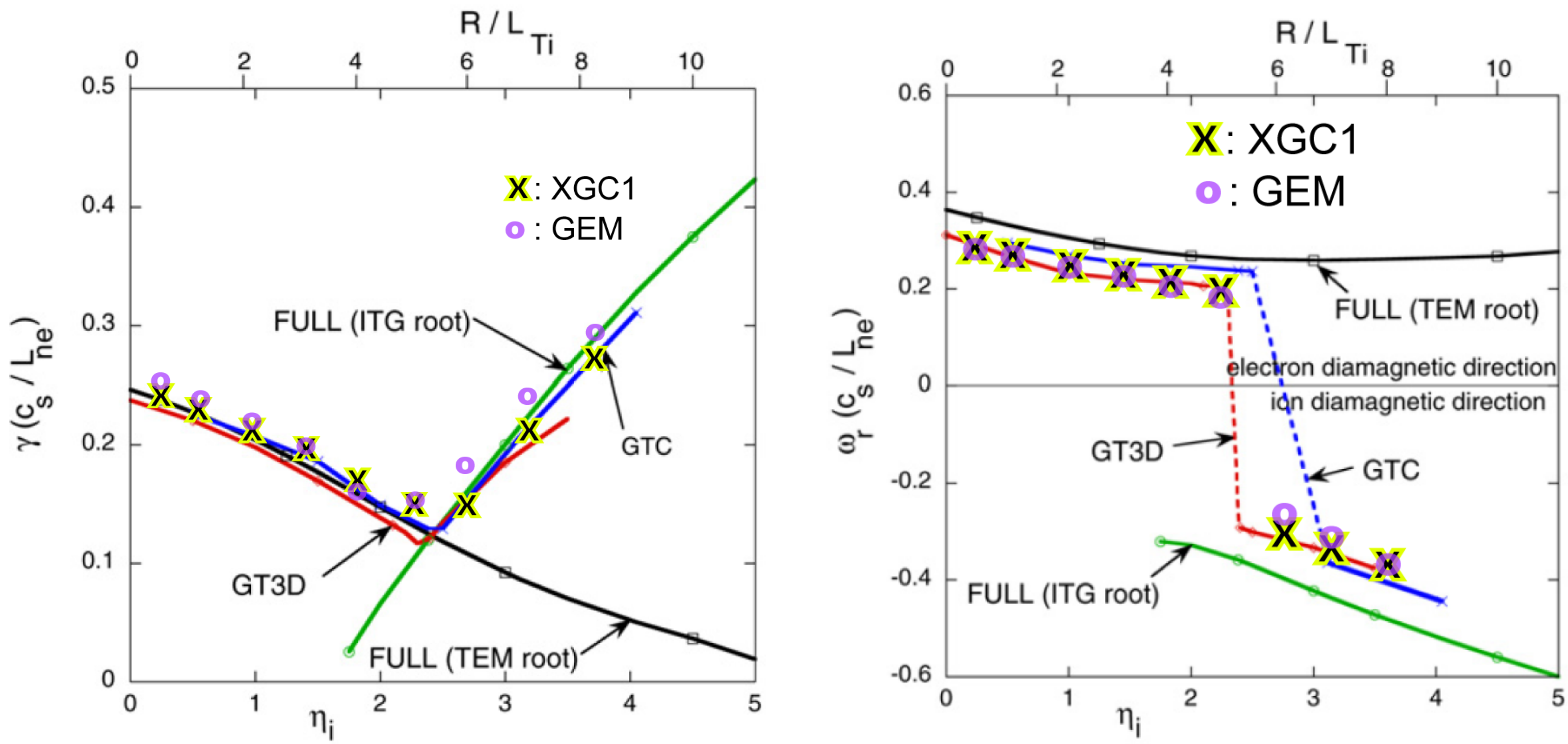
Differene between fluid codes and XGC:

Fluid: Er is calculated from force balance on assumed plasma profile and V_θ.

XGC: E_r, V_θ and pedestal profile are kinetically self-organized quantities [e.g., flux shape affects $E_r(r)$, $V(r)$, $n(r)$]

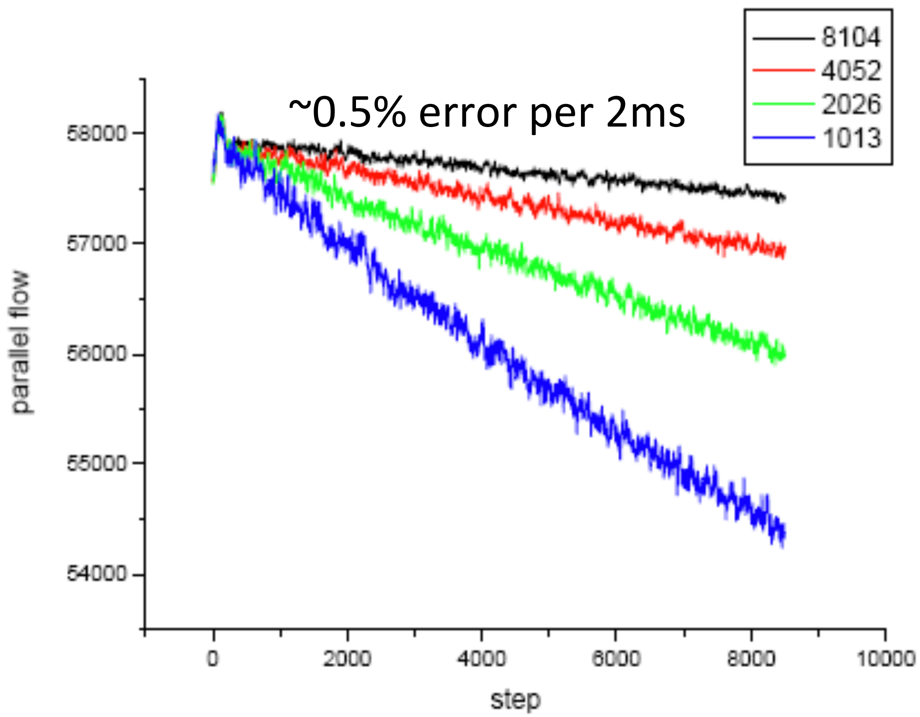
XGC1 has been verified in various ways [Ku et al, NF09]

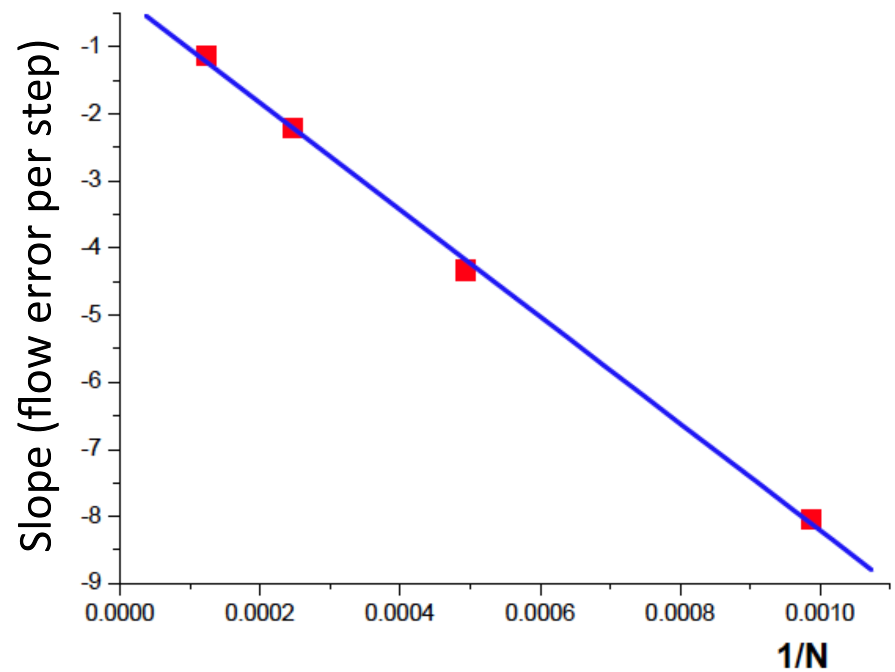
Recent multi-codes cross-verification of ITG-TEM transition in δf method (GTC/FULL/GT3D/XGC1-δf/GEM)



- Original figures from Rewoldt, et. al. Computer Phys. Comm. (2007)
- The cross-verification updated in Holod and Lin, PoP 20, 032309 (2013)

At a practically strong rotation speed, conservation of momentum in XGC1 has been verified. Mostly affected by particle noise ($\propto$1/N)





Simulations started with a canonical Maxwellian.

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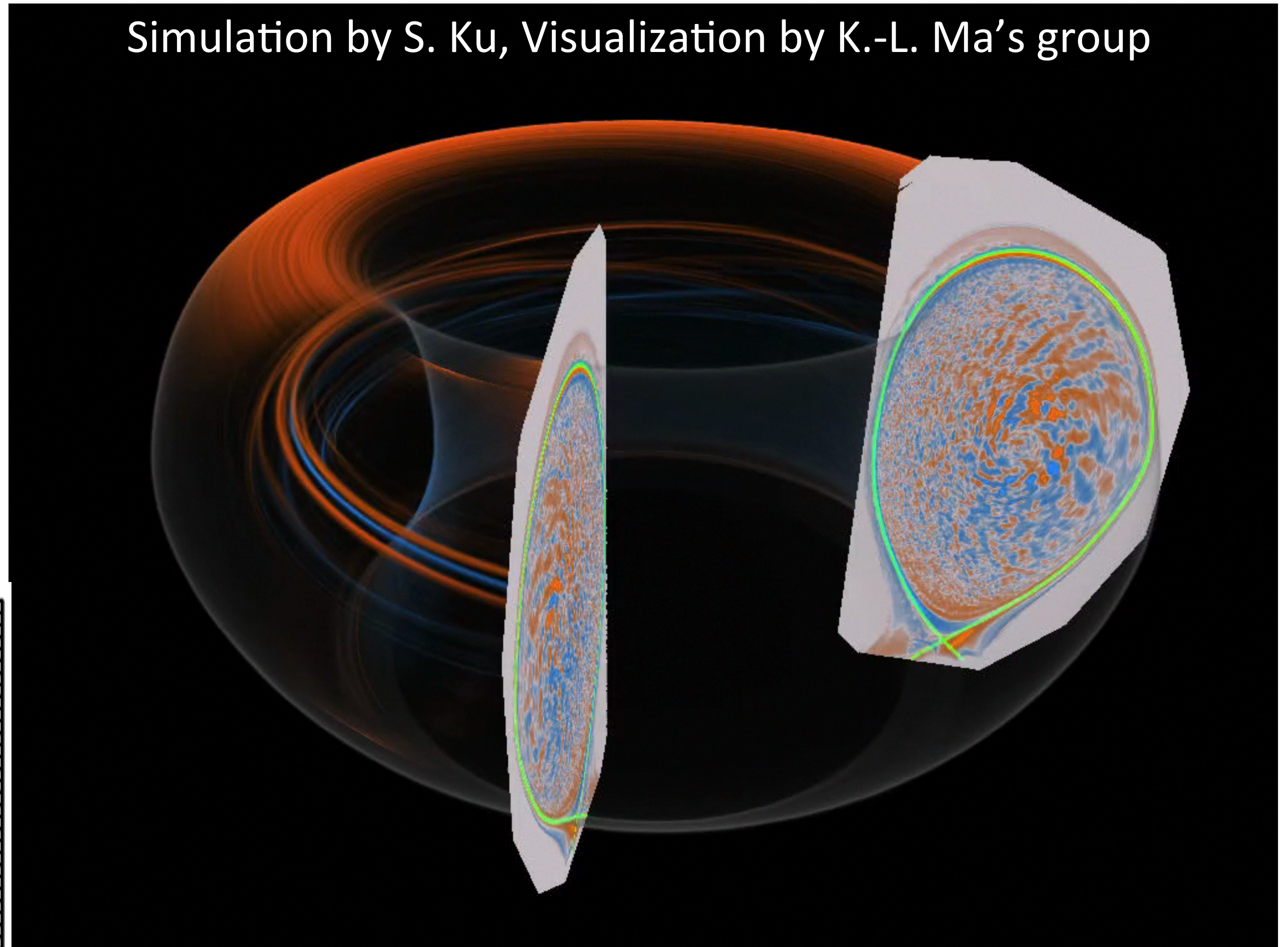
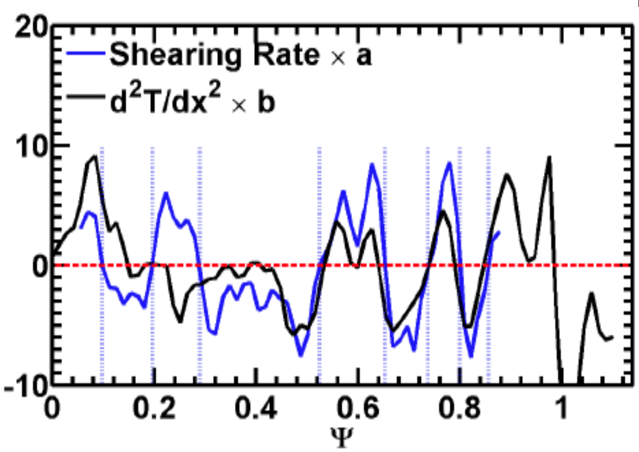
2) Full-f ion physics in XGC1

- Gyrokinetic ions, Adiabatic electrons, and Monte Carlo neutrals recycled at wall
- Realistic boundary condition: Φ_W=0. No core-edge boundary.

→Self-organization of a flux-driven plasma-ITG-neutrals system

- Plasma and turbulence evolve together until stiff SOC where power balance is maintained
- Self-organization through ExB zonal flow and GAM exicitation





2D neutral particles evolve consistenly with plasma

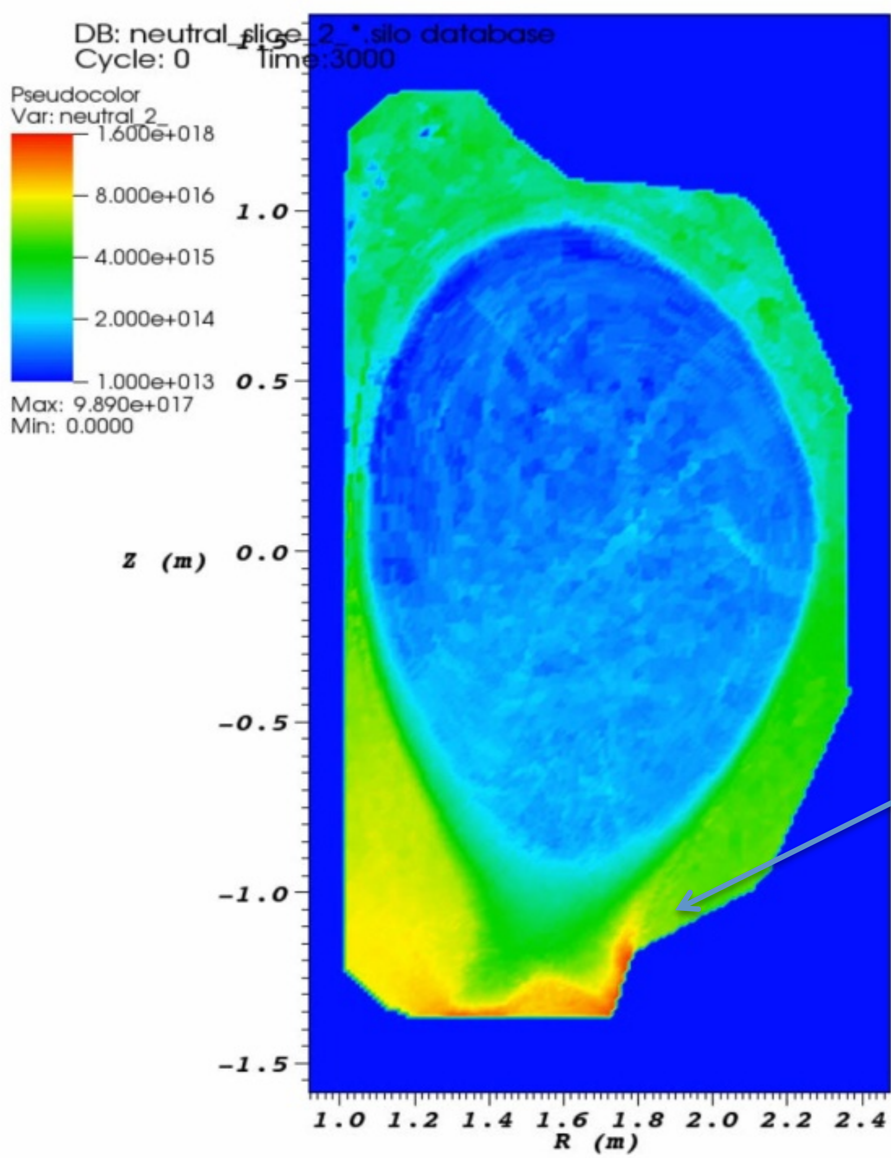
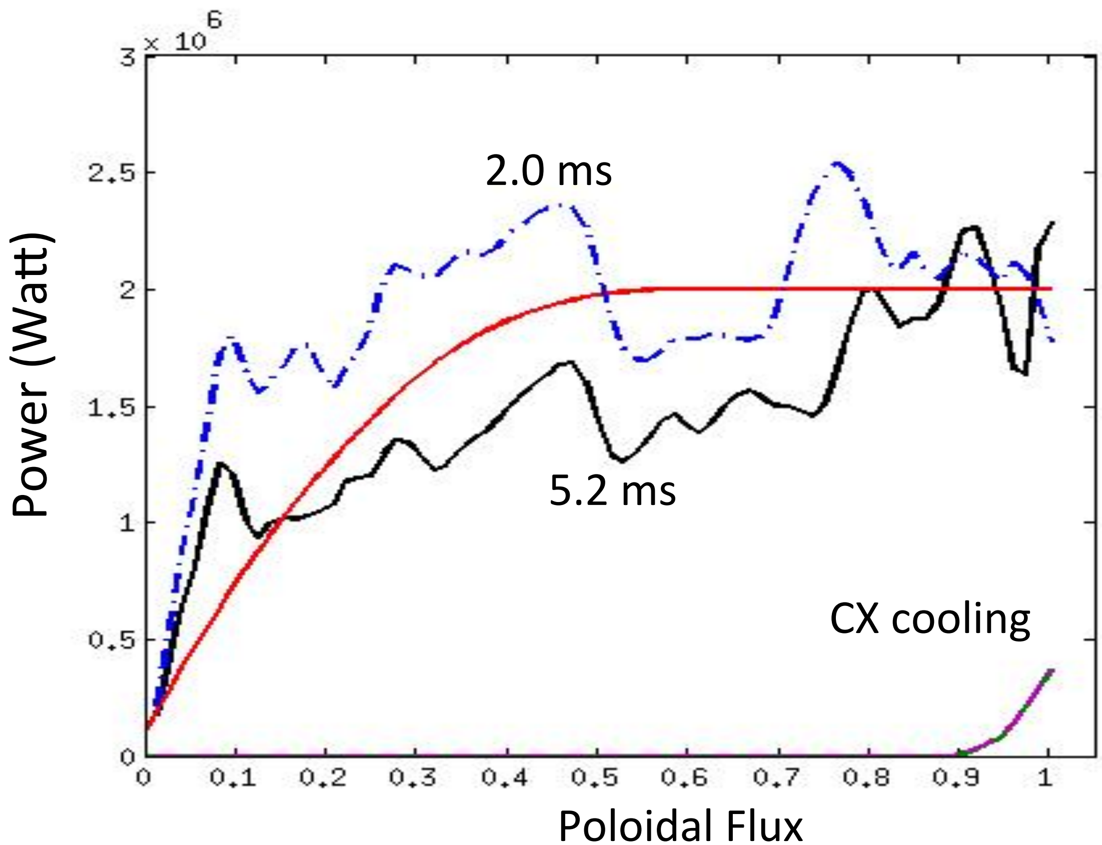


Figure by D. Stotler

Logarithmic plot of 2D deuterium neutral atom density in a DIII-D plasma

(showing that that the neutral source is peaked at the divertor targets, as determined by the poloidal profile of XGC ion losses to wall).

Power balance is a turbulence time-scale concept



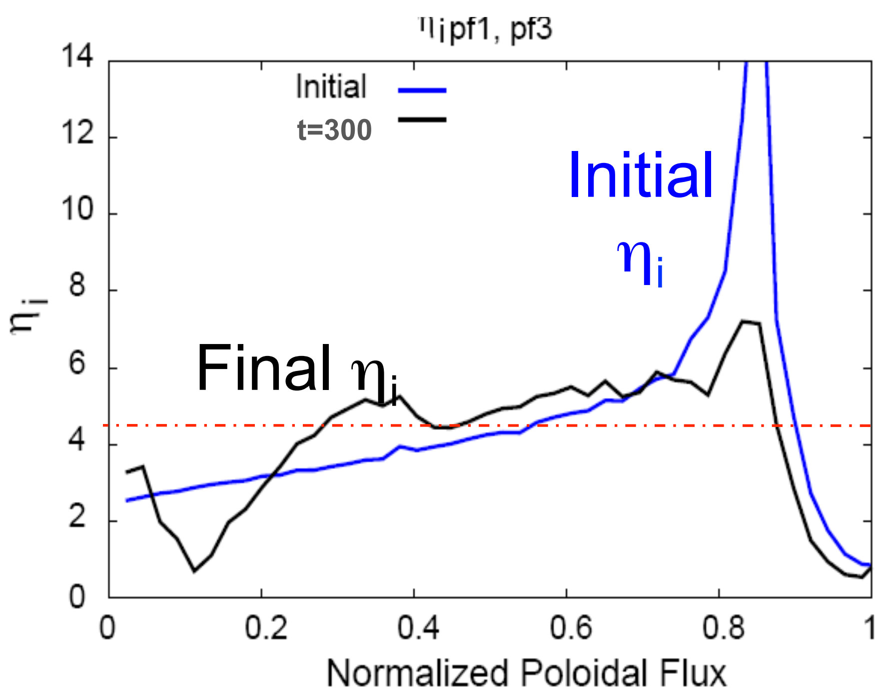
- Meso scale GAM and limit-cycle appear to set the power-balance time.
- During the power balance, plasma and turbulence continuously seek for SOC.

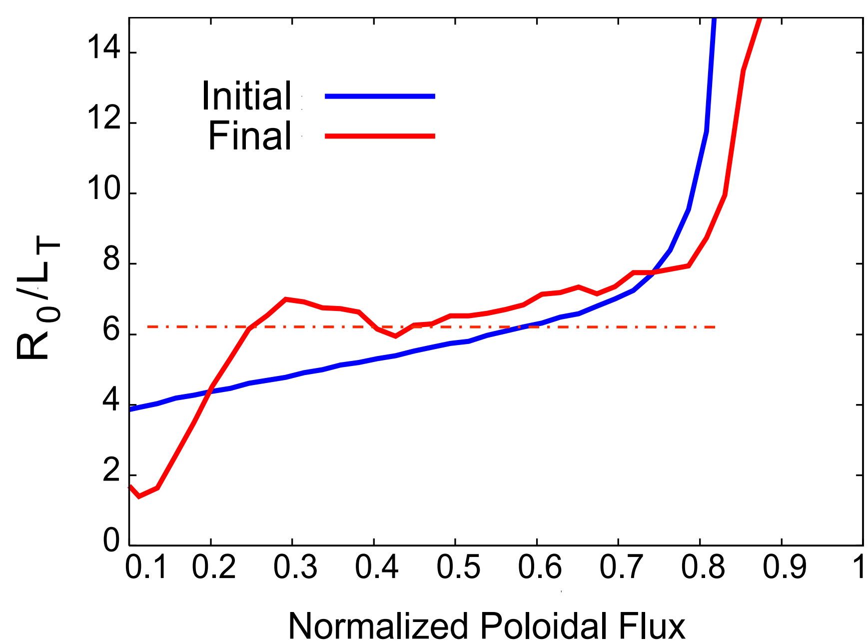
Red: Total heating power
Purple: Charge exchange cooling at 2.0 ms
Green: Charge exchange cooling at 5.2 ms

- Neoclassical
- ITG turbulence
- Neutrals
- Ti-Te Collision

XGC1 evolves T_i in stiff self-organized criticality

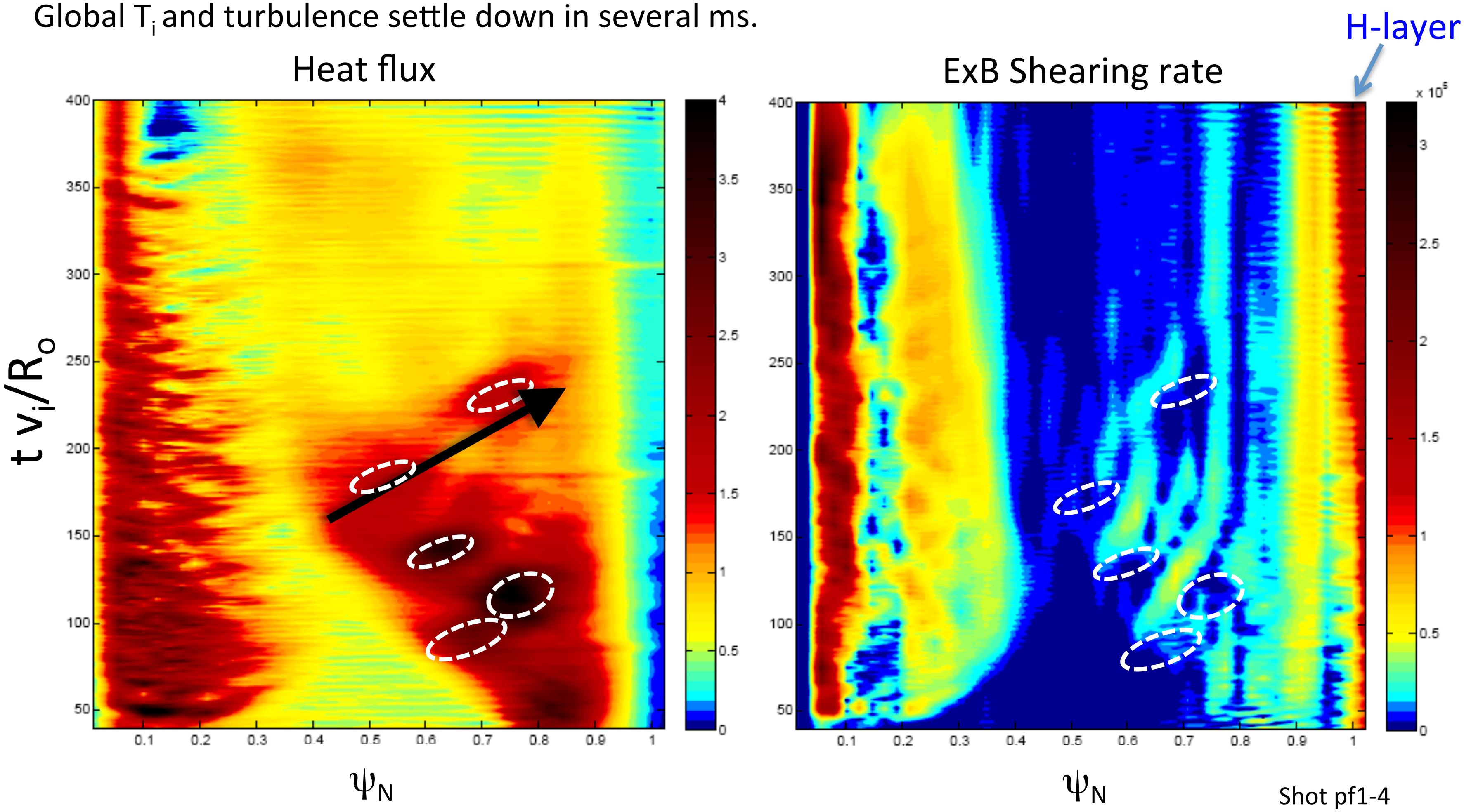
- TRINITY, TGYRO, etc: "Scale separation assumption. Turbulence simulation in small regions of the space-time grid, embedded in a coarse grid on which fluid transport equations are evolved" [M. Barns et al, PoP2010]
- XGC1 studies turbulence and transport physics without scale separation, together with heat/torque source, wall-loss and neutral particles
- Turbulence in XGC1 yields a "stiff" self-organized T_i profile. **Edge T_i determines core T_i.**



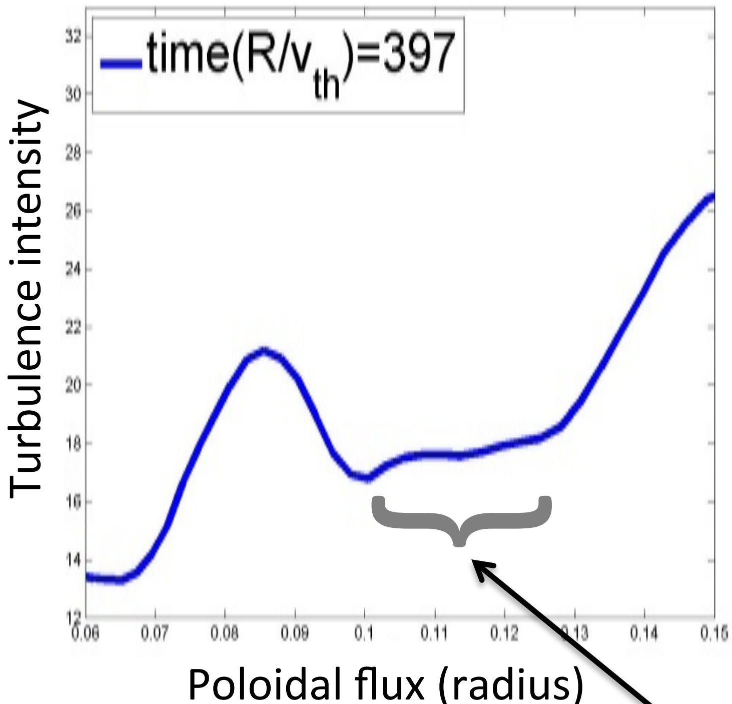


Self-organizing interaction between outward heat bursts by ITG turbulence and E'xB control of turbulence

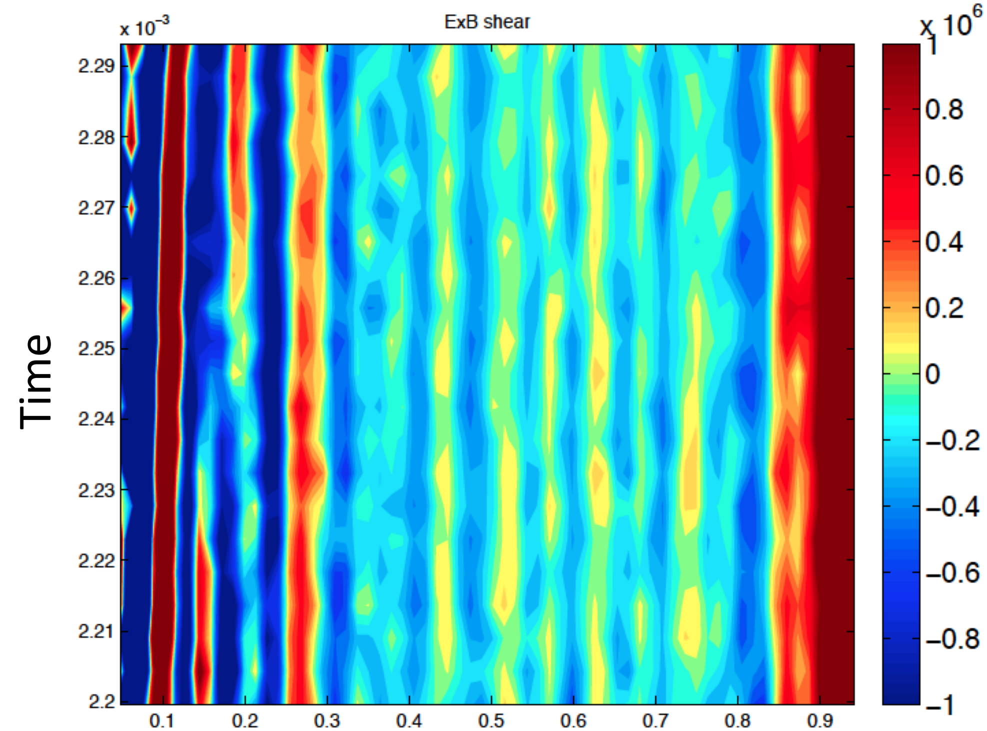
- Self-organizing interactions in the ω-k-x-t space can be clearly seen in the bursty initial stage
- Similar interactions at smaller scale exists at later time in the form of avalanche and zonal layers
- Temperature perturbation information at edge propagates to core in this fashion, taking <3ms in DIII-D: cold/hot pulse experiment, propagation speed ~ 0.3 km/s ~ 1.7 $\rho_{(i,0.6)} v_{(i,0.6)} / R_0$ ~ 0.4 V_*
- Global T_i and turbulence settle down in several ms.



Self-organization and ExB Staircase



ExB shearing rate in the final time window



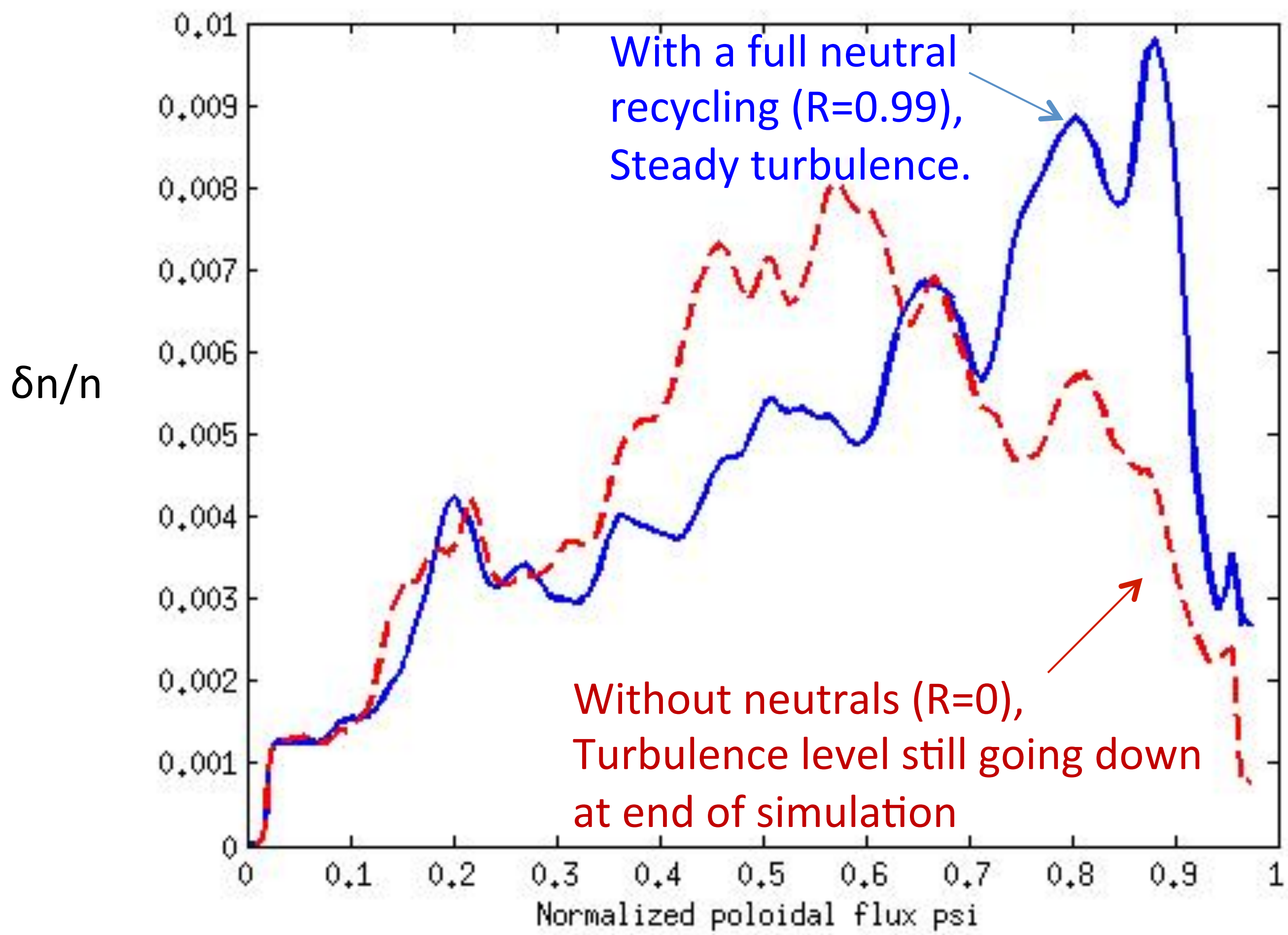
Poloidal flux (radius)

Drop in turbulence intensity: sign of internal transport barrier?

Strongly sheared ExB layer

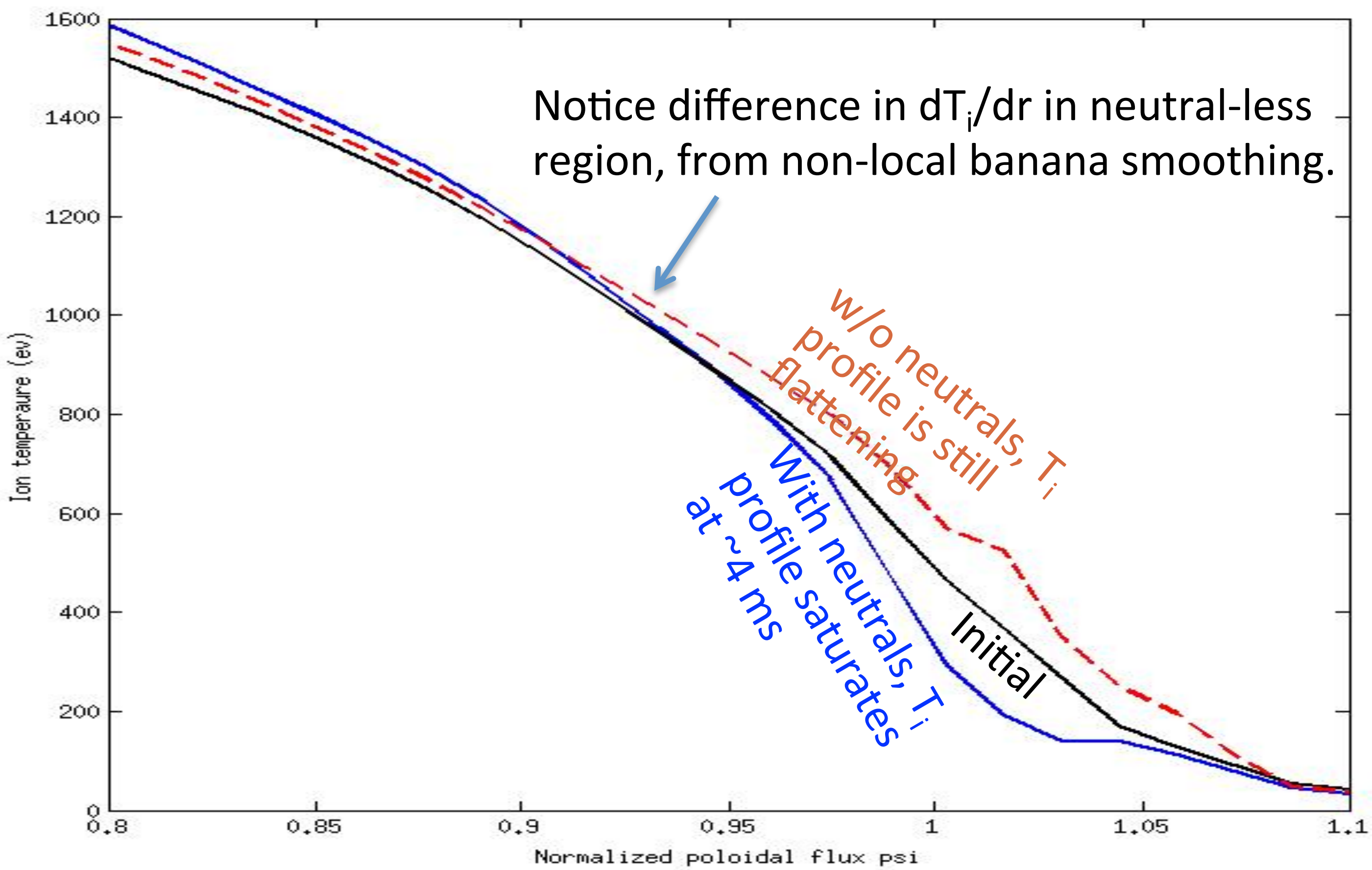
XGC1 showes that ITG turbulence is sensitive to neutral atomic physics

- Cooling of T_i in pedestal slope → A higher turbulence drive (η_i) at pedestal top
- Damping of ExB shearing rate by neutrals



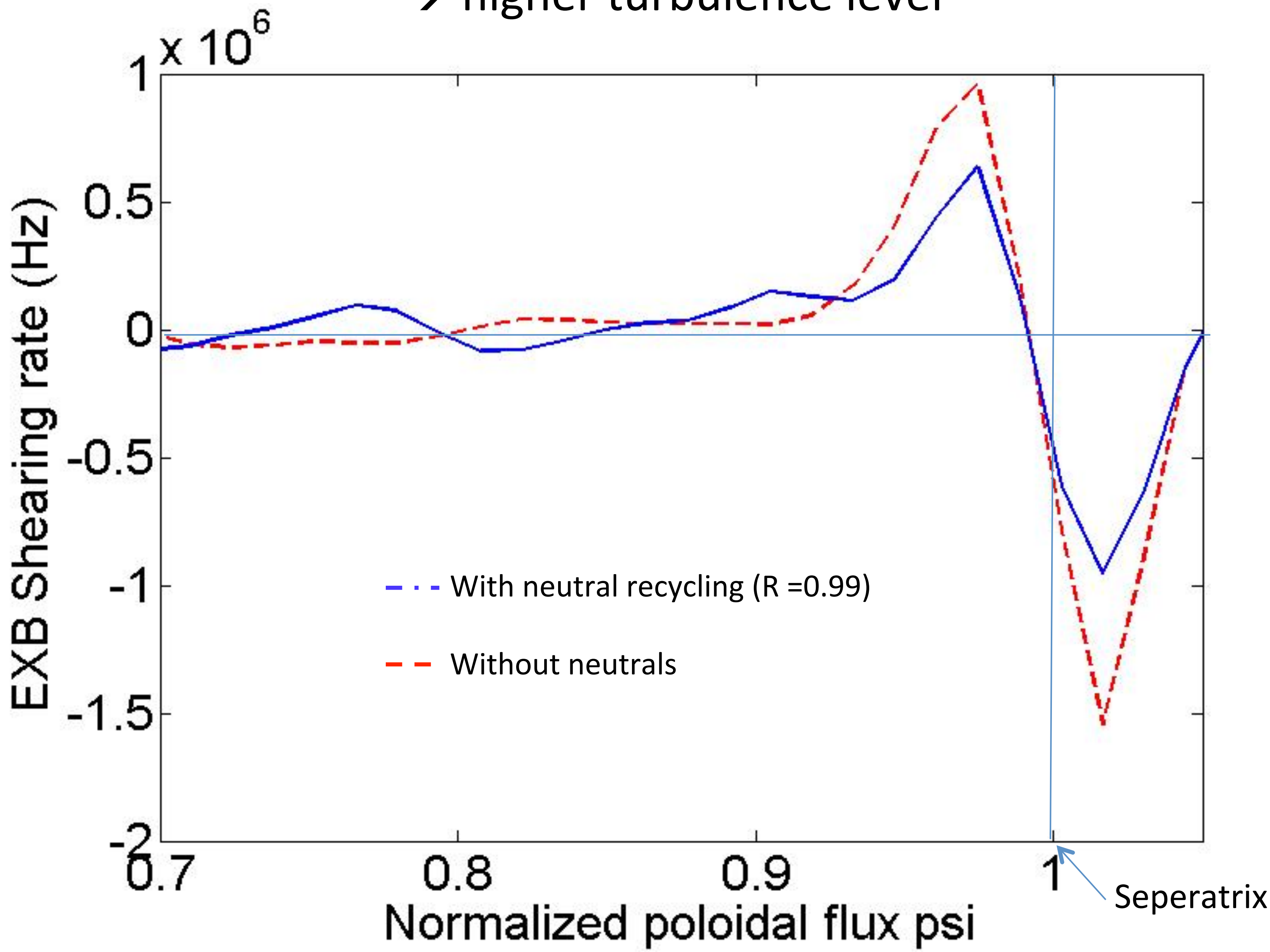
Neutral particles at outer part of pedestal affect η_i at pedestal top from the ion orbit smoothing

- Edge T_i profile saturates at steeper gradient with neutral particle recycling
- Maintaining adequate η_i and high edge ITG turbulence is difficult without neutrals



EXB shearing rate is weaker with neutrals in the edge pedestal

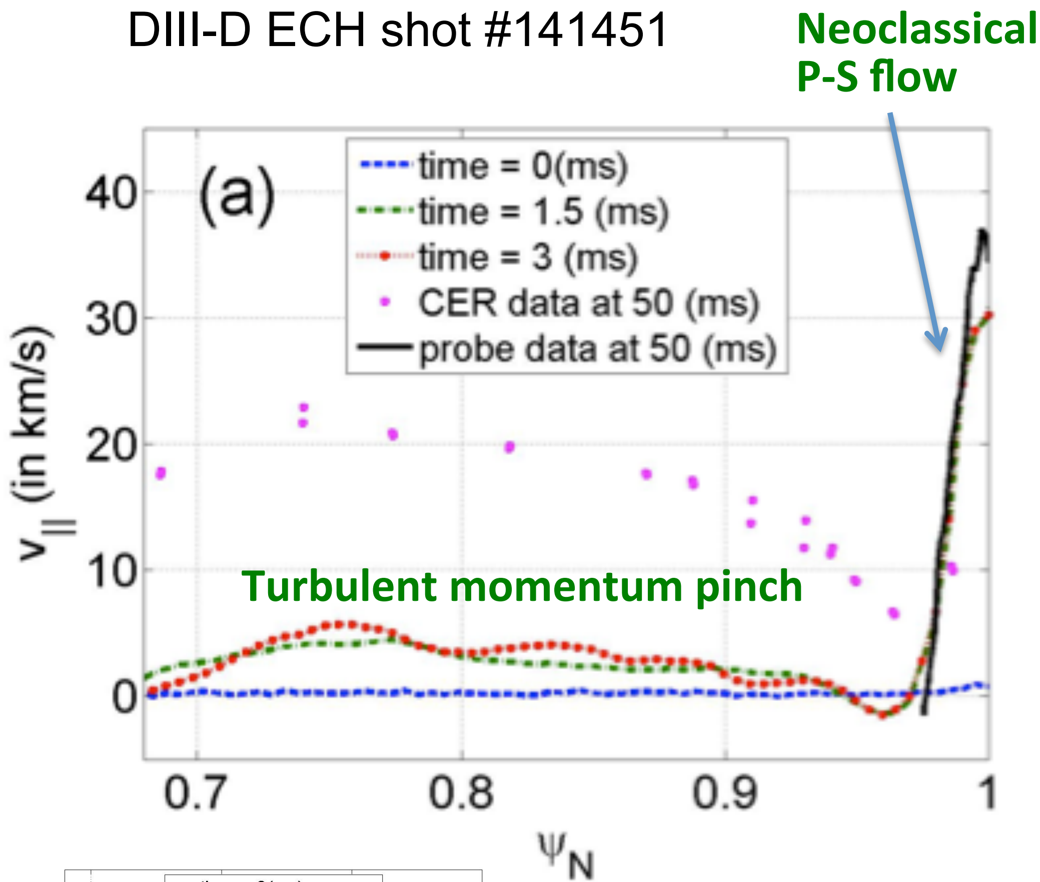
→ higher turbulence level

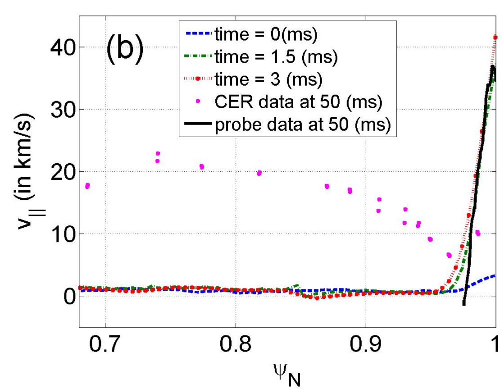


Edge rotation source and inward momentum pinch

- Detailed experimental measurement exists [S. Muller, PRL & PoP, 2011]
  - Conventional fluid Reynolds stress could not explain experiment
- Full-f XGC1-produced edge rotation profile and inward momentum pinch speed, agreeing with experimental data
  - Edge rotation is from PS flow + orbit loss
  - Momentum pinch: In addtion to the conventional theory, full-f interaction between turbulence and neoclassial orbits is needed

DIII-D ECH shot #141451





No turbulence → no momentum pinch. But, the edge rotation persists (P-S flow + orbit loss).

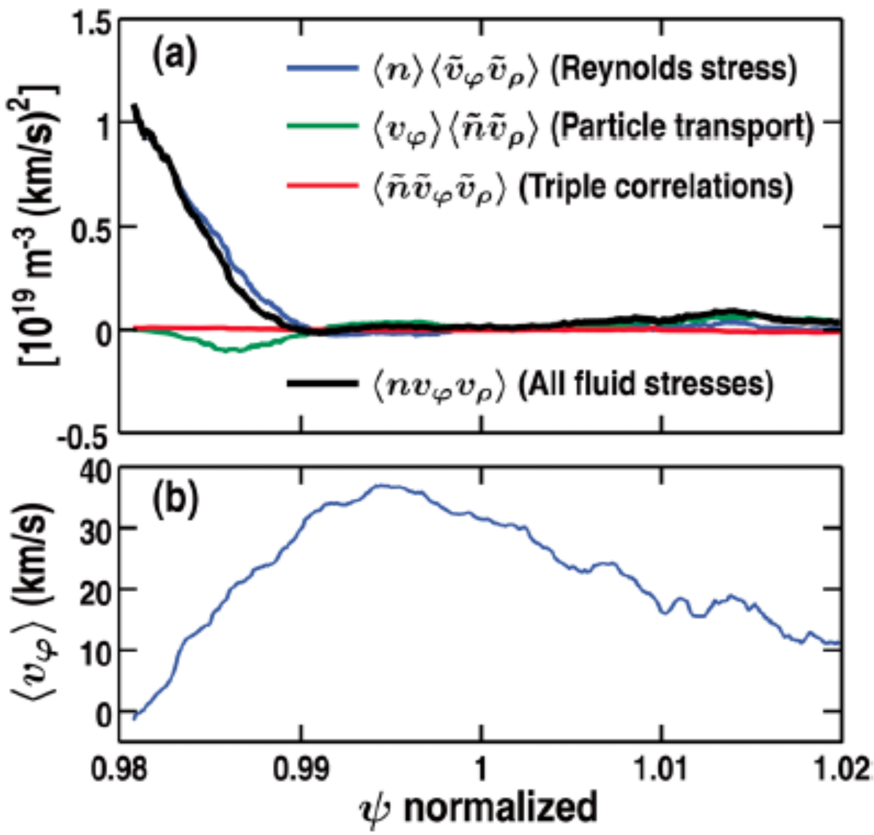
Validation of the edge momentum source and the inward momentum flux in DIII-D edge plasma

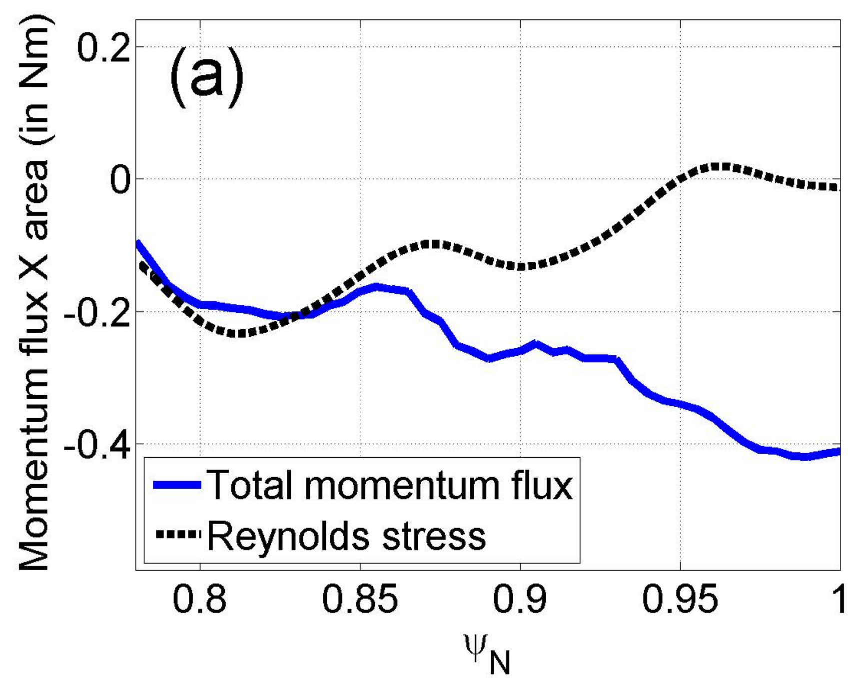
Experiment (Muller et al., 2011)

- Edge momentum source seen
- Measured turbulent Reynolds stress cannot explain either edge momentum source or inward momentum transport

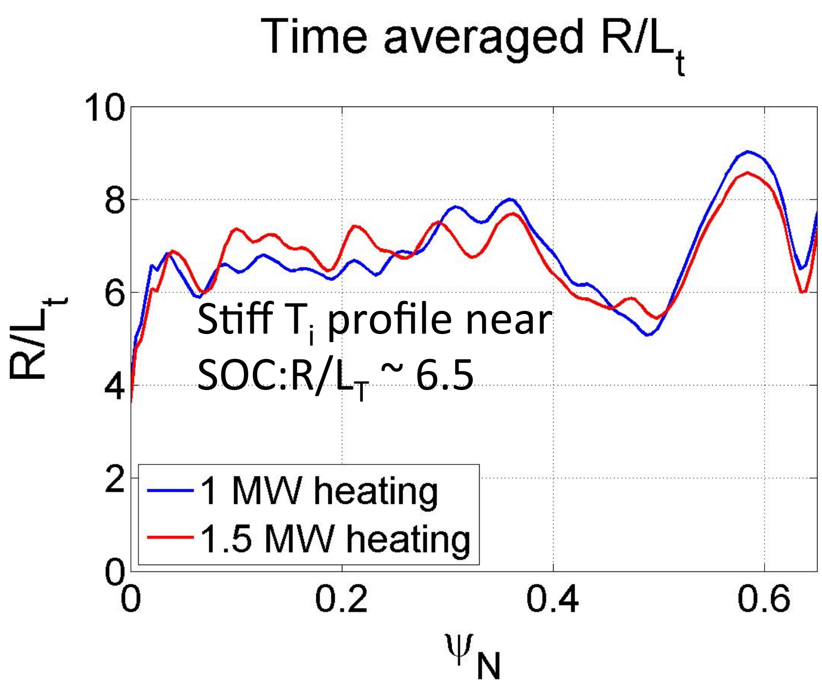
XGC1 simulation (Suh et al., 2013)

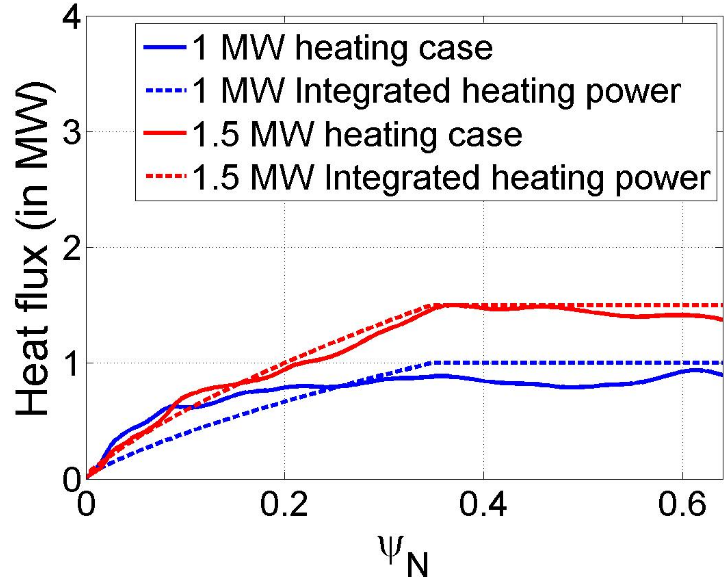
- Momentum source is observed and identified to be from neoclassical physics
- Total momentum flux from full-f ITG + neoclassical orbilts is inward, with a correct magnitude.





Ion transport in the KSTAR core agrees with stiff ITG turbulence + Neoclassical

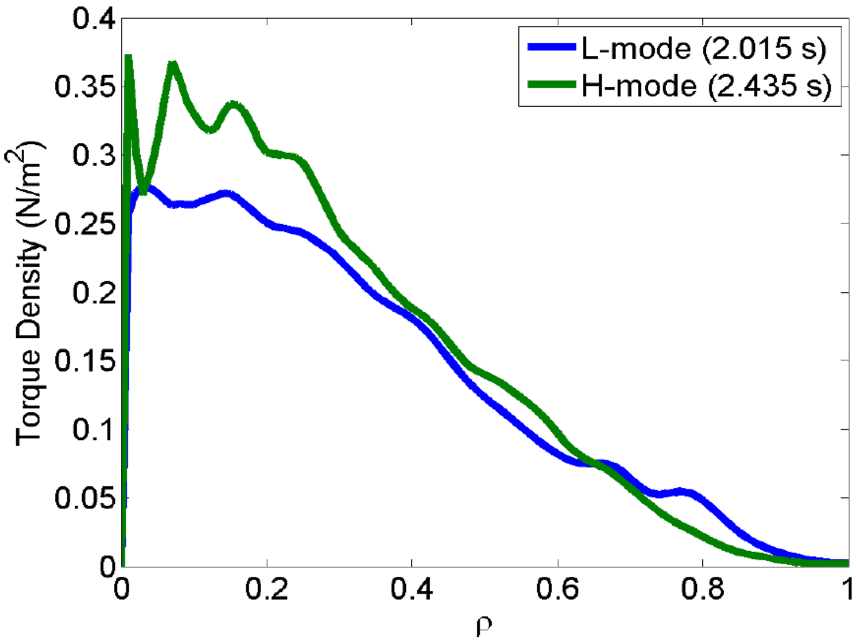




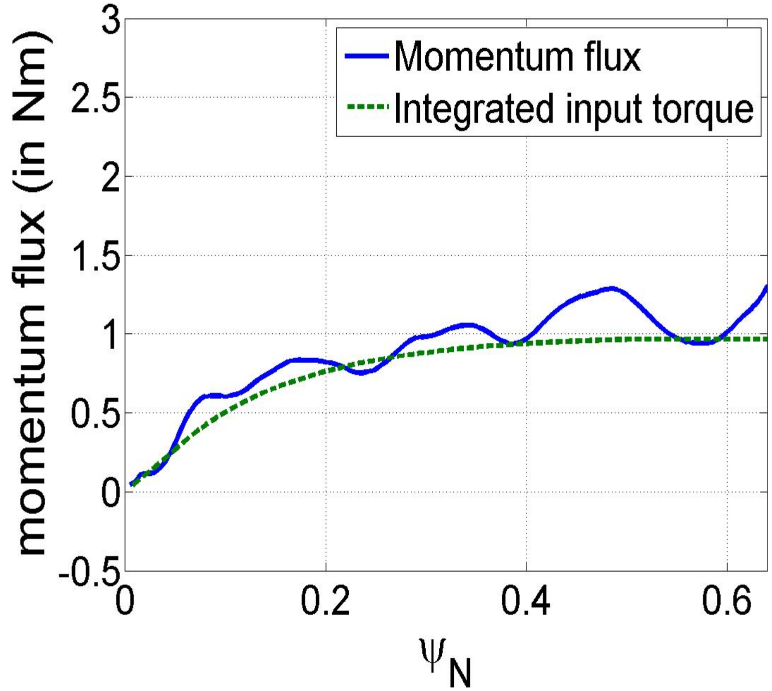
- H mode shot #5681 at time= 2.48 s
- NBI heating power is 1.5 MW: 1 or 1.5 MW to ions examined
- Less heating power keeps similar R/L_T → stiffness
- Heating region : ψ_N=from 0 to 0.35

Momentum transport is also consistent with ITG turbulence in KSTAR H-mode

Experimental torque profile from NUBEAM



XGC1 simulation results



- Total torque ~ 0.95 (Nm) (from NUBEAM analysis)
- Graph shown here is for 1.5MW ion heating case

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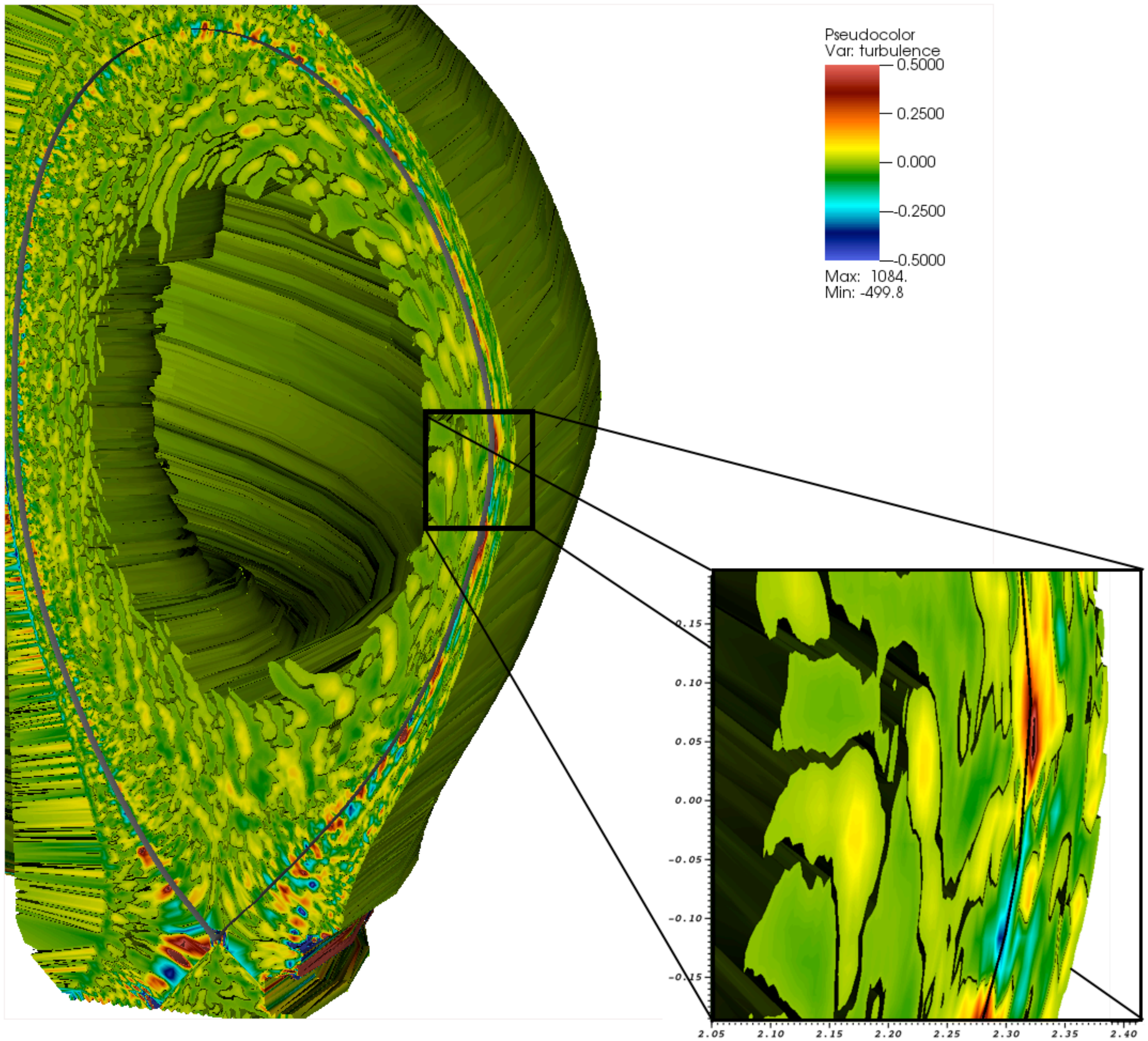
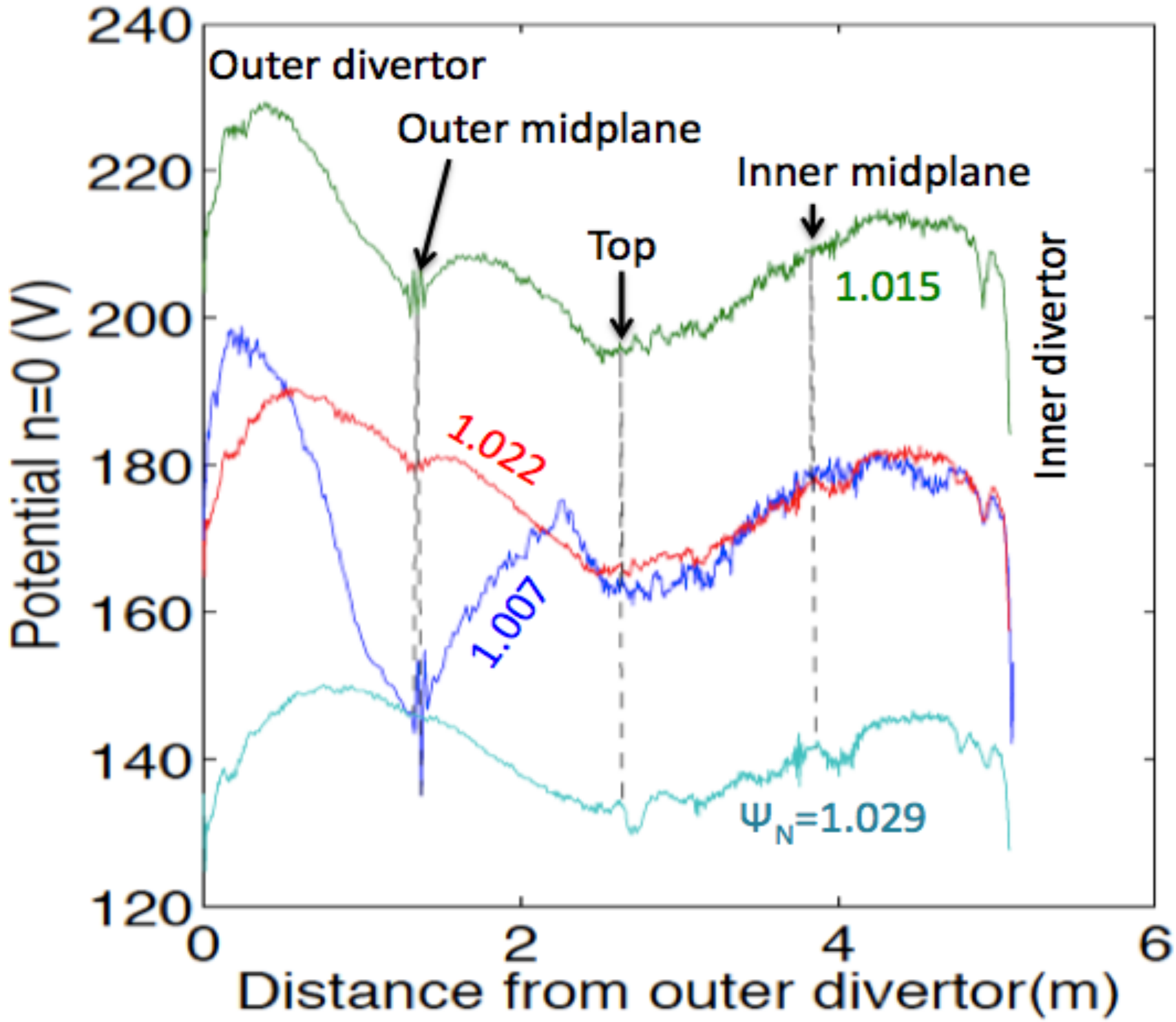
4) Summary

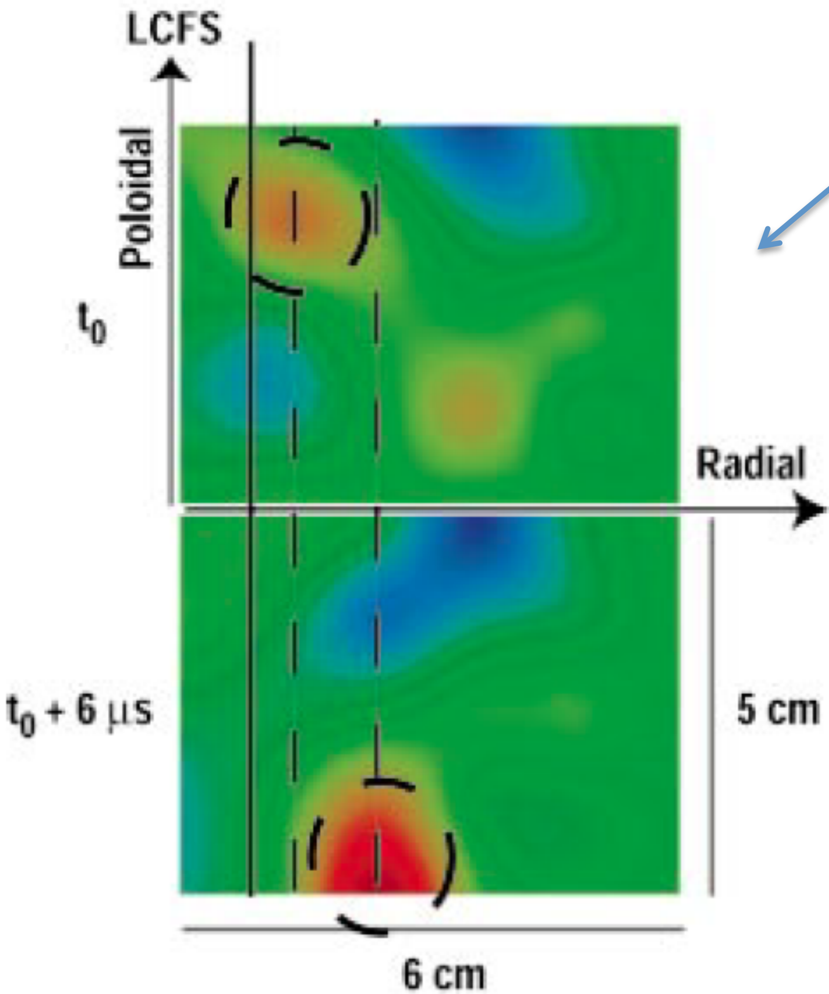
2. Kinetic electrons → nonlinear coherent structures



Poloidal potential variation in the scrape-off layer

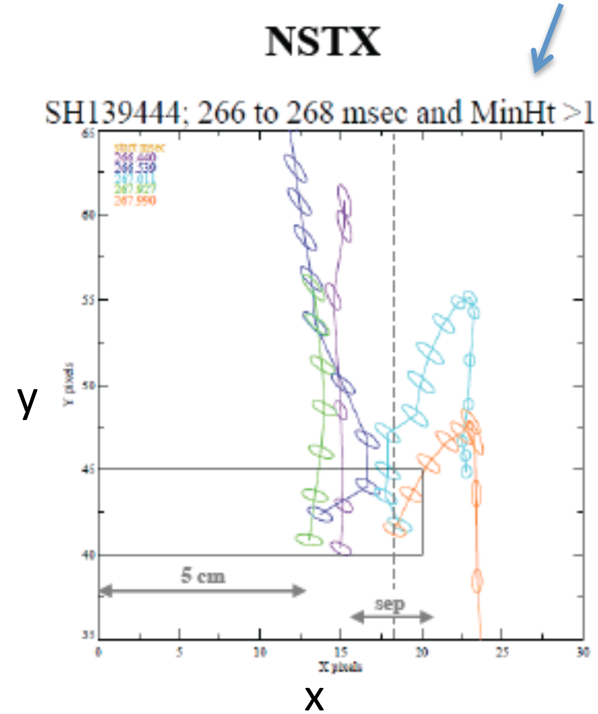


Examples of H-mode blobs in experiment



Boedo et al. PoP 2011, BES
Soon after H-transition in DIII-D

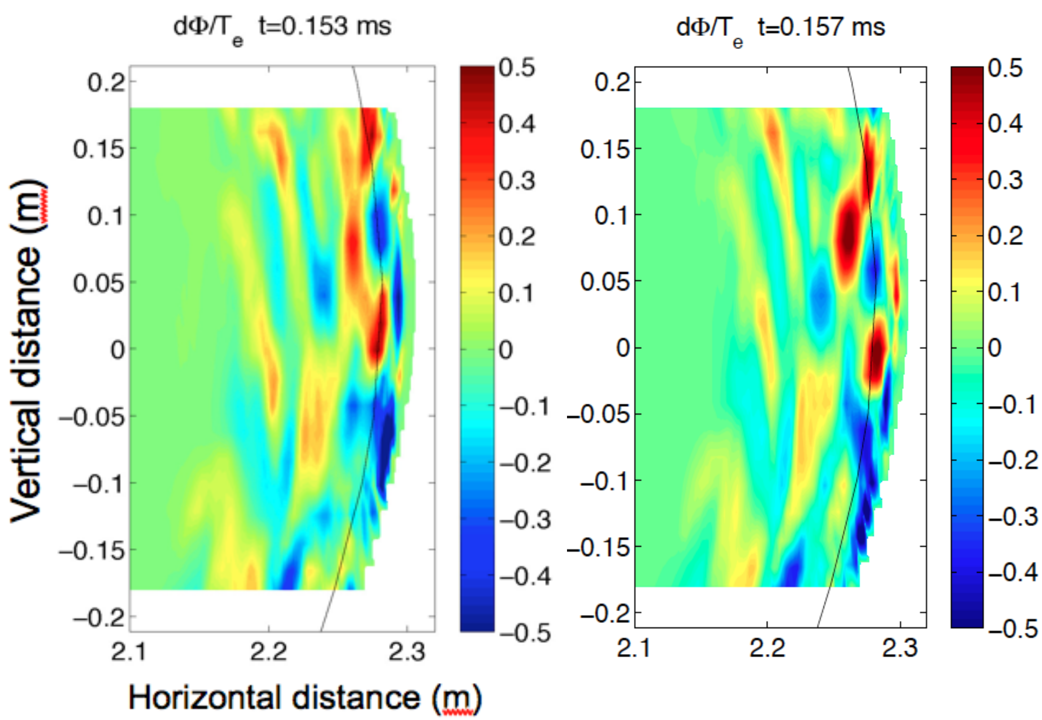
- In H-mode, blobs move more rapidly in the poloidal direction than the radial direction
- In L-mode, the blob motion is more noticeable in the radial direction (see D'Ippolito, Myra, Zweben PoP 2011)



Myra et al.
TTF 2012
NSTX L-mode

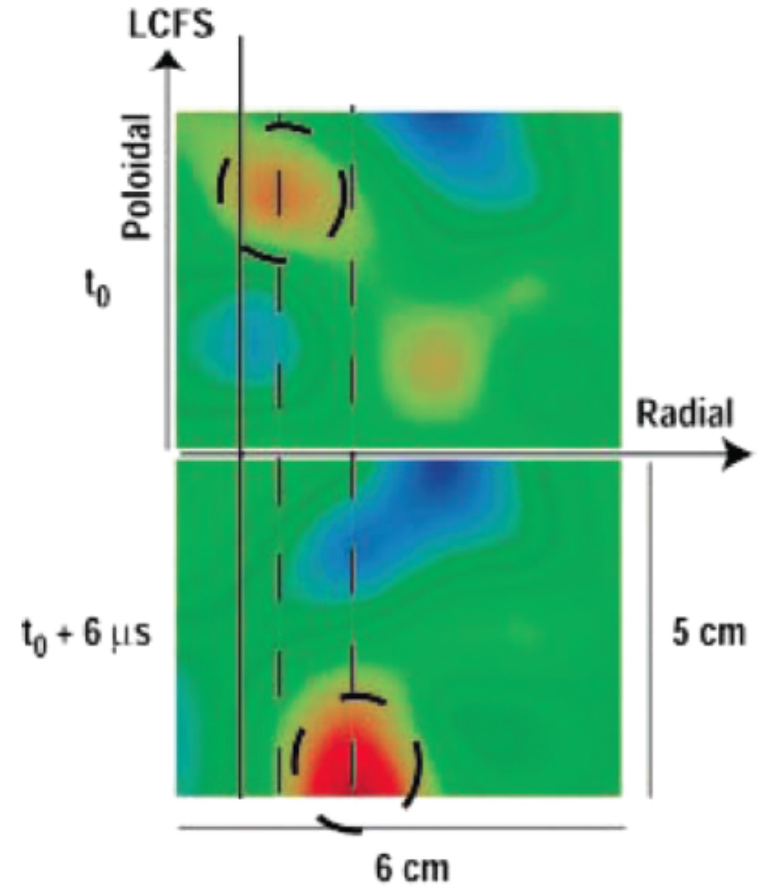
Time-slice figures of $e\delta\Phi/T_e$ from XGC1, zoomed into the outboard midplane of a diverted tokamak edge (DIII-D).

- Blobs are generated by shearing action by EXB flows near separatrix
- Blobs move outward across the separatrix into scrape-off



Gyrokinetic blobs in XGC1, 2013

As blobs move out, they also move downward by a several cm in 4 µs.

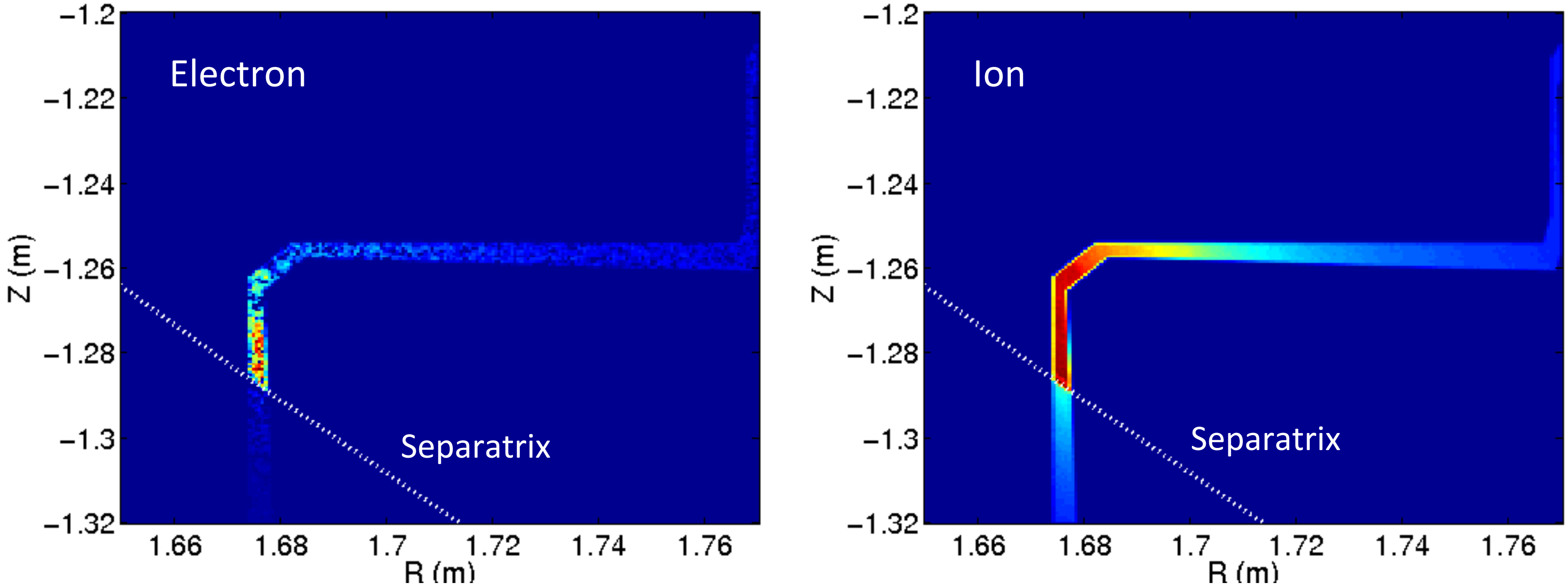


Blob motion in DIII-D, 2013

[Boedo et al, BES]

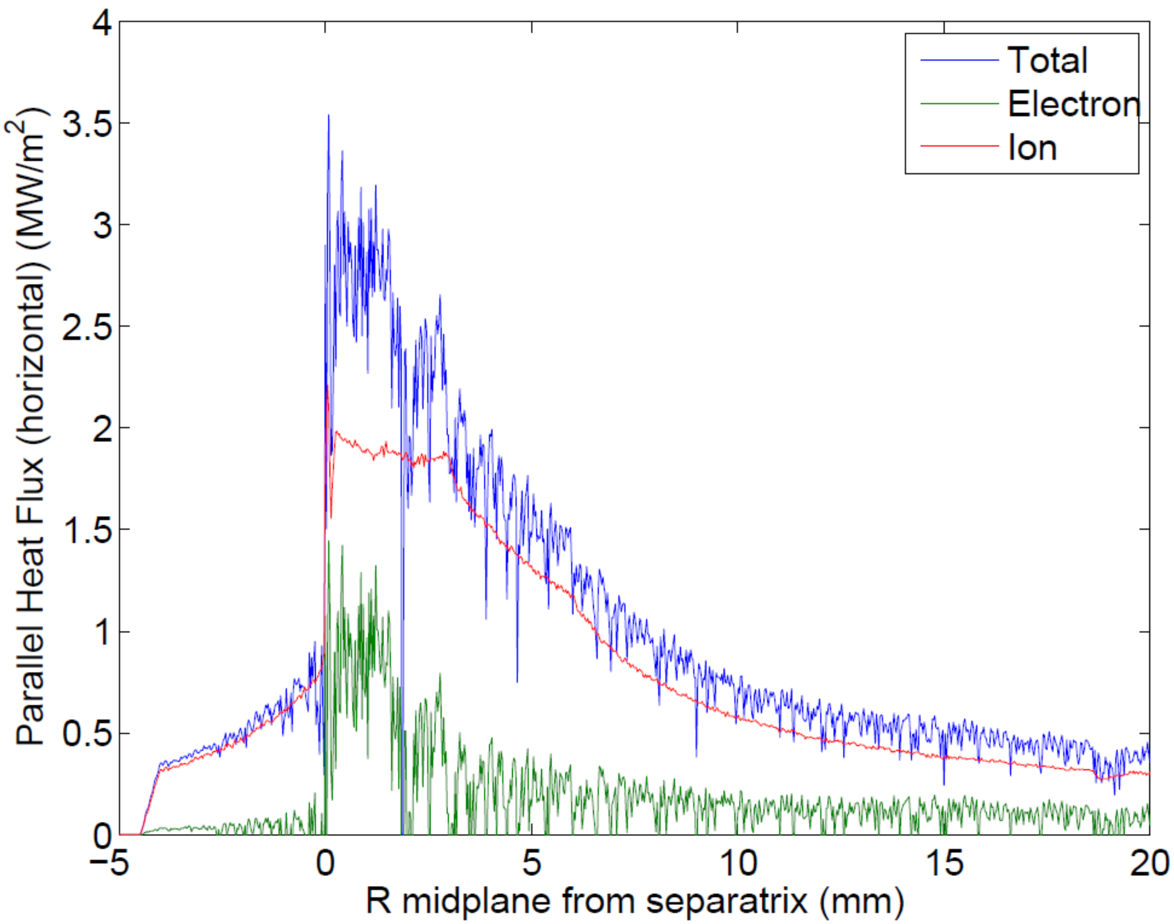
XGC1 measures heat load footprint on a given divertor configuration.

Heat deposition profile on outboard DIII-D divertor



- With nonlinear Coulomb collisions and neutral recycling
- Ions show wider heat flux footprint than electrons

Heat-load width, measured in ψ_N and mapped back to outside midplane

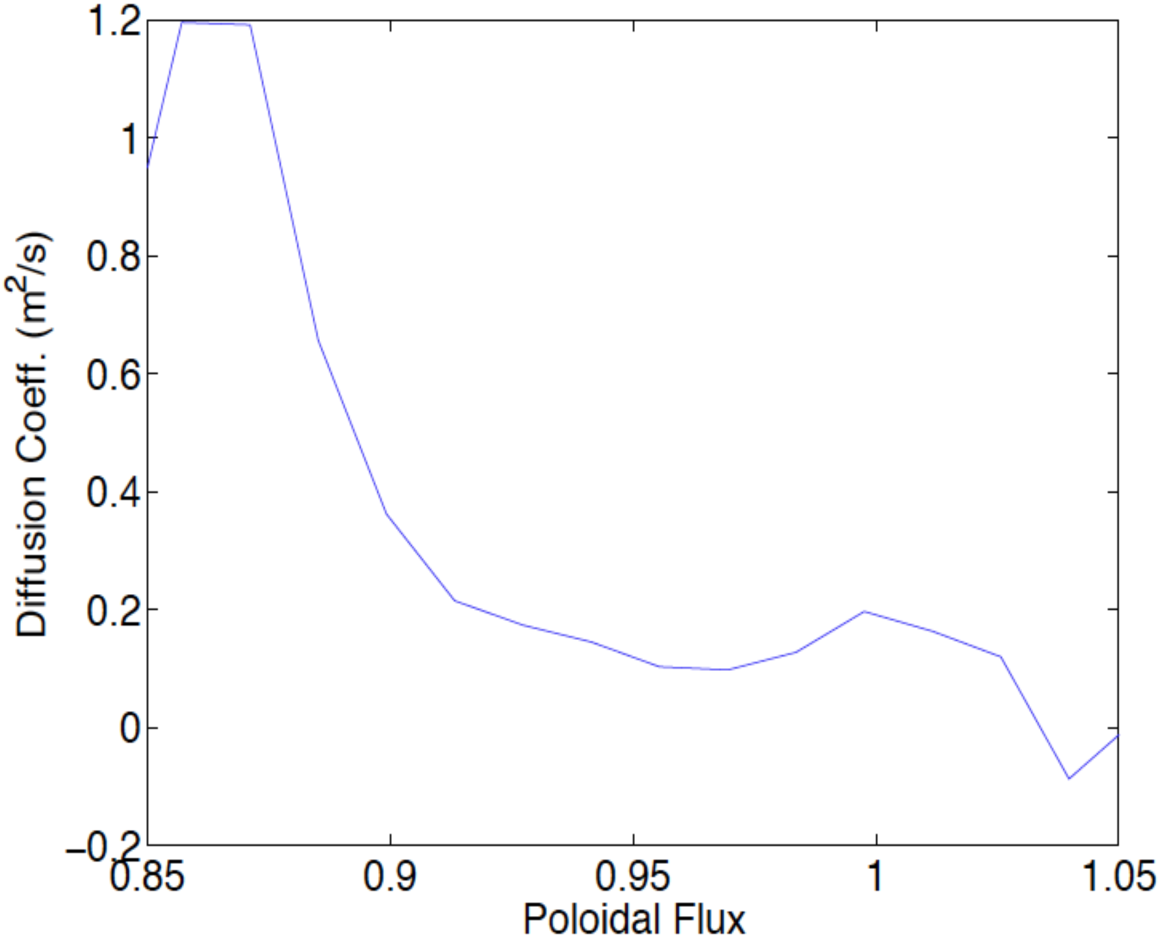


- λ_q =4.4 mm: Shorter than the average blob size (~1cm)
- Closer to ion banana width (~3mm)

  → 1/I_p type scaling in present-day tokamaks, as found from experiments and XGC0 [2010 DOE JRT Report]and Goldston
- At high B, such as ITER, will the blobs saturate the 1/I_p type scaling?
  - We already see such a sign

Effective radial particle diffusivity in H-mode pedestal stays small even with blobs → Indication of inward particle pinch?

(Preliminary result)

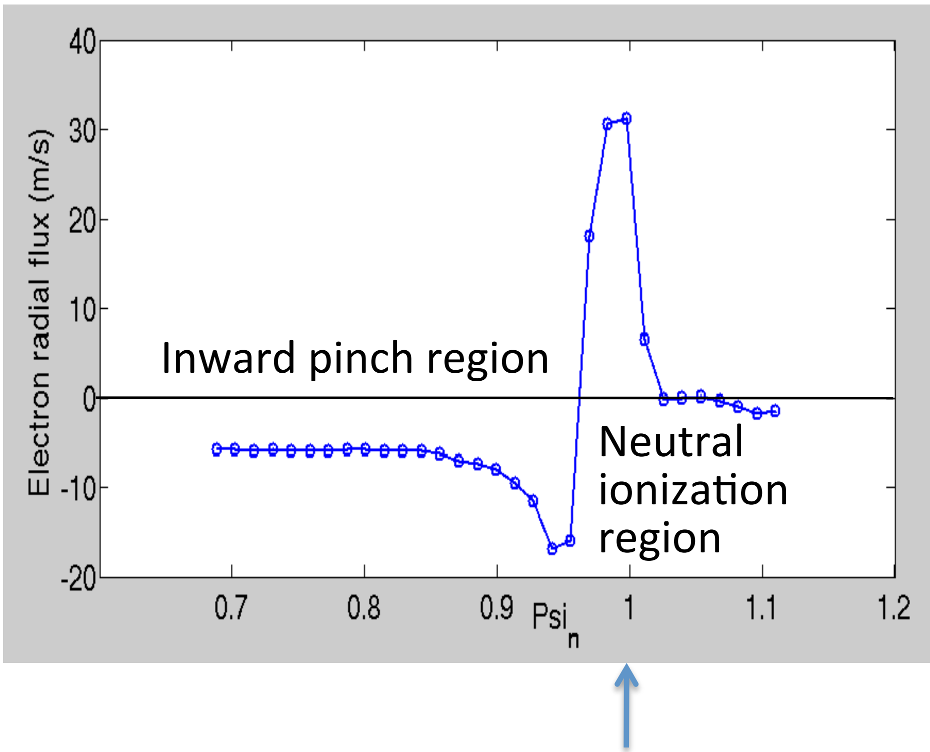


Inward particle pinch is found!

(preliminary result)

Electrostatic edge turbulence yields inward particle pinch in the presence of neutral particles!

Electron radial transport



Magnetic separatrix

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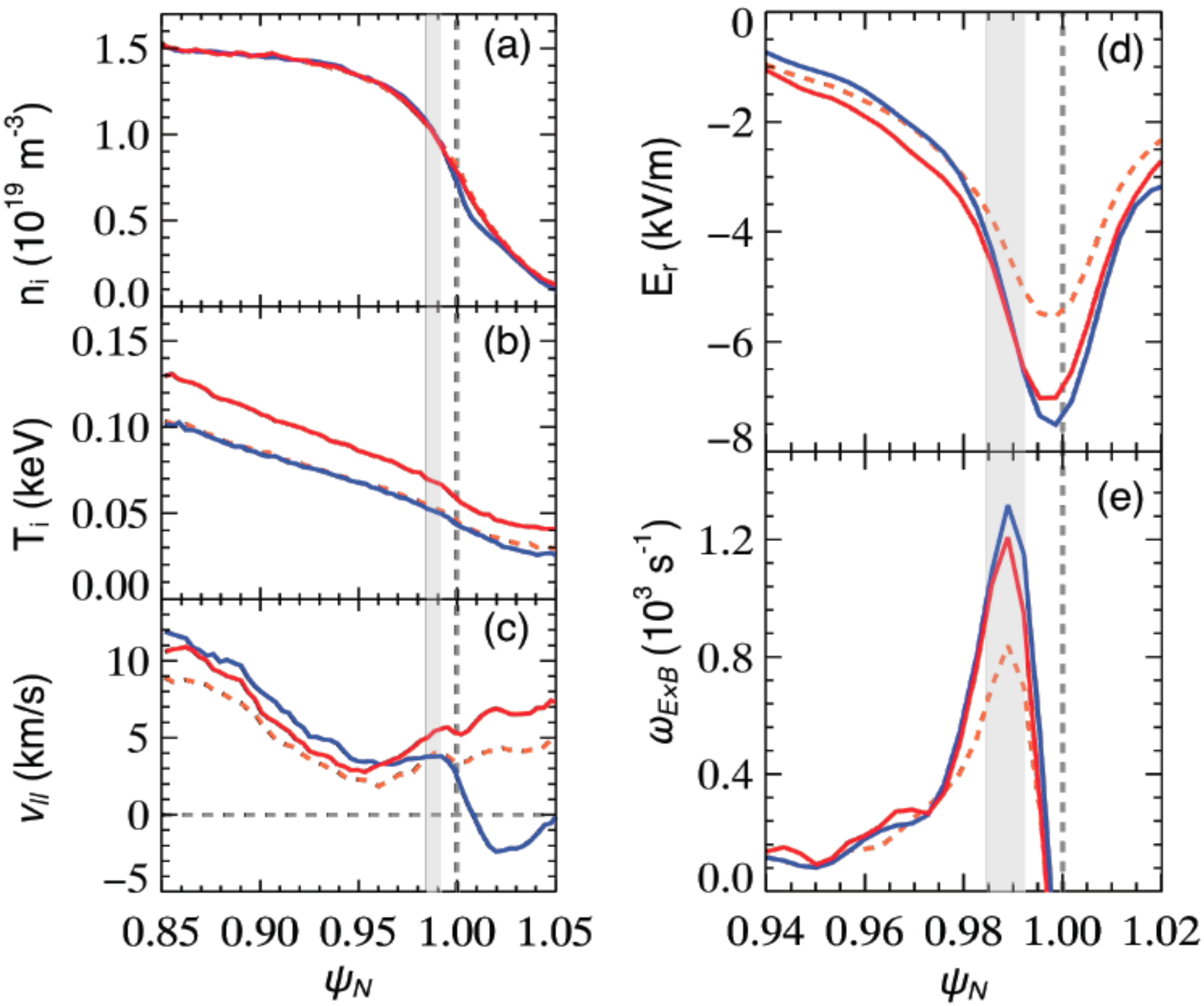
Starting the quest for the L-H transition physics

- XGC1 is starting to study physics related to L-H transition
- There are two types of experimental observations w.r.t. L-H transition
  - Neoclassical ExB shearing rate is corelated with L-H transition

    S.M. Kaye et al., Nucl. Fusion 51, 113109 (2011)
    D.J. Battaglia et al., Nucl. Fusion 53, 113032 (2013)
    Others
  - Vorticity merging and secondary oscillation are observed before and at L-H transition: HL-2A (IAEA2012) & others
- Both types of observations are supported by XGC codes
- **XGC1 will attempt a gyrokinetic L-H transition in 2014**

XGCn's provide evidences that neoclassical ExB shearing rate is correlated with $P_{L\rightarrow H}$

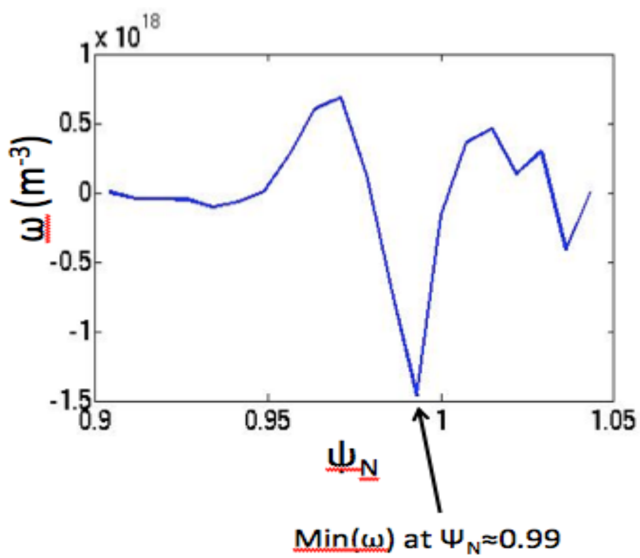
[Fiture from Battaglia et al., NF 2013 on NSTX plasma]

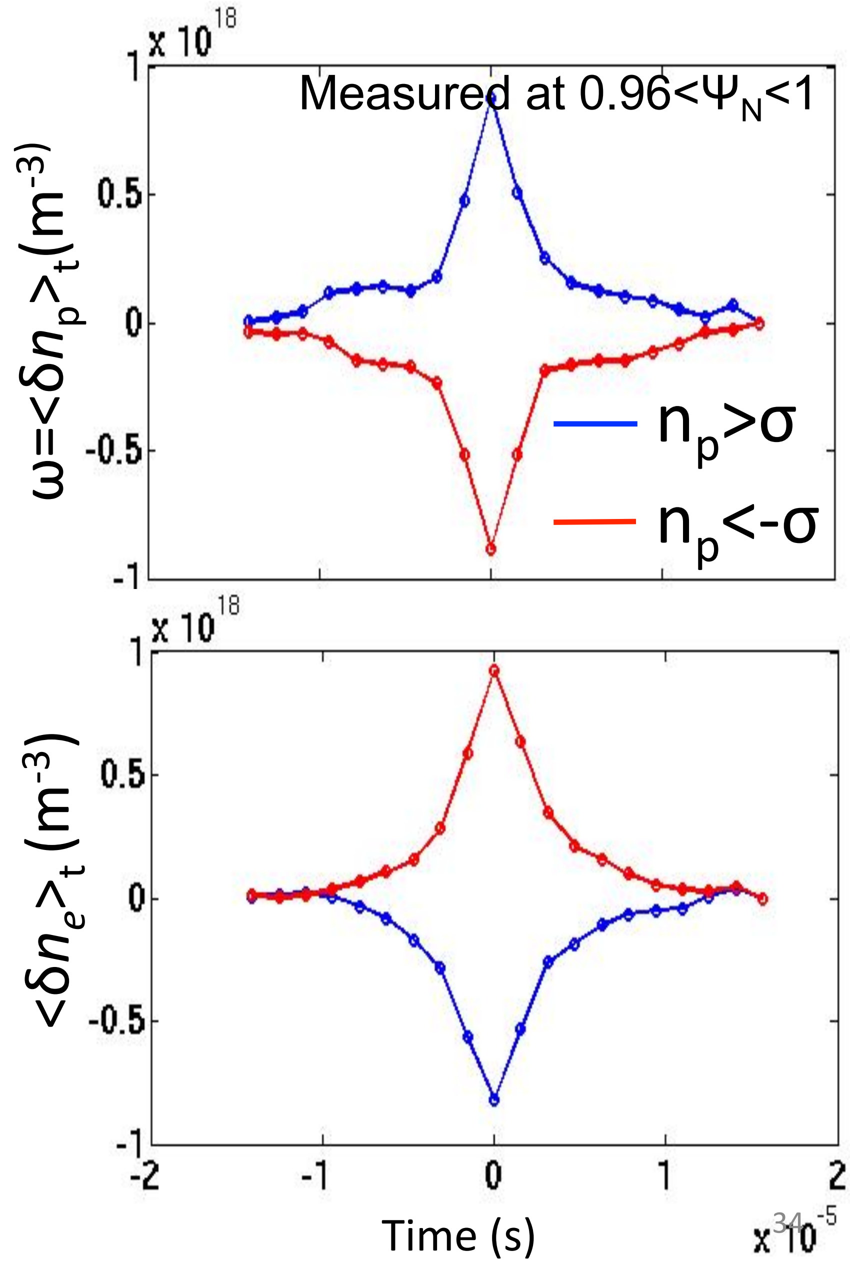


- Experiment: Smaller R_X requires 30% higher $P_{L\rightarrow H}$ and torque
- XGC0: At 30% higher power and torque, the ExB shearing rate is similar to larger R_X plasma
- XGC0 finds
  - Anomalous $D=\chi=0.1\ m^2/s$ is needed to match experimental profiles.

XGC1 has verified vorticity merging in edge pedestal

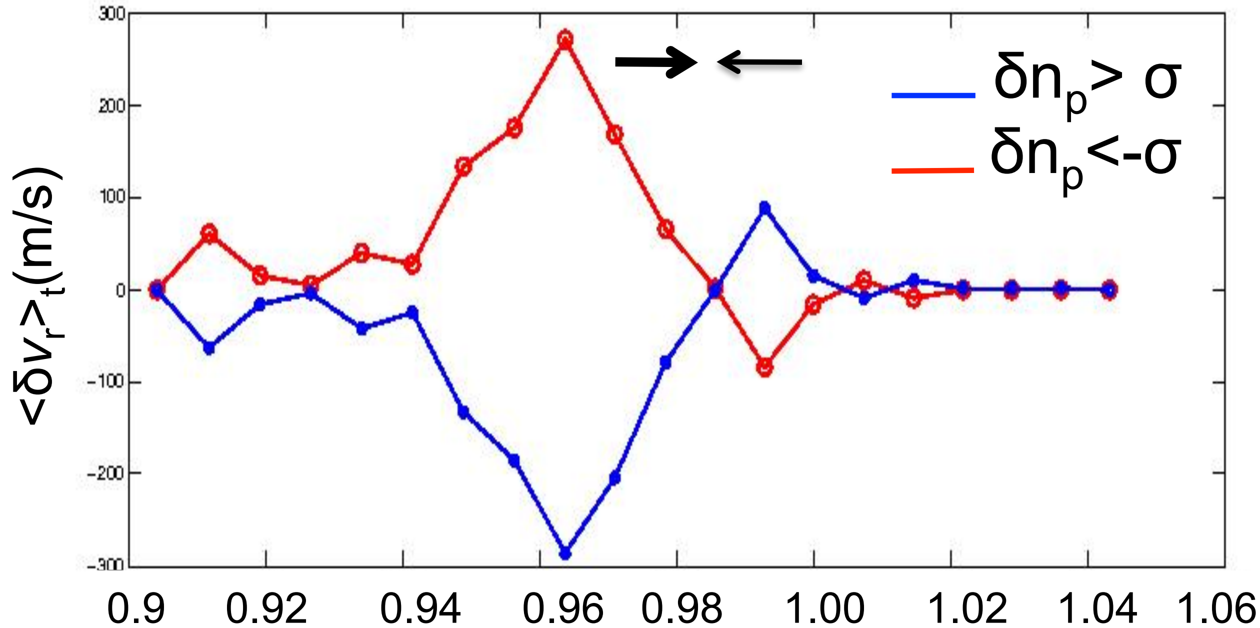
- Vorticity merging to a surface just-inside the separatrix is observed in XGC1 with both
  - adiabatic electrons (ITG turb.) and
  - kinetic electrons (ITG + TEM + Resistive + other drift waves)
- and in both
  - L-mode (affects L-H transition?)
  - H-mode (affects hysterisis?)

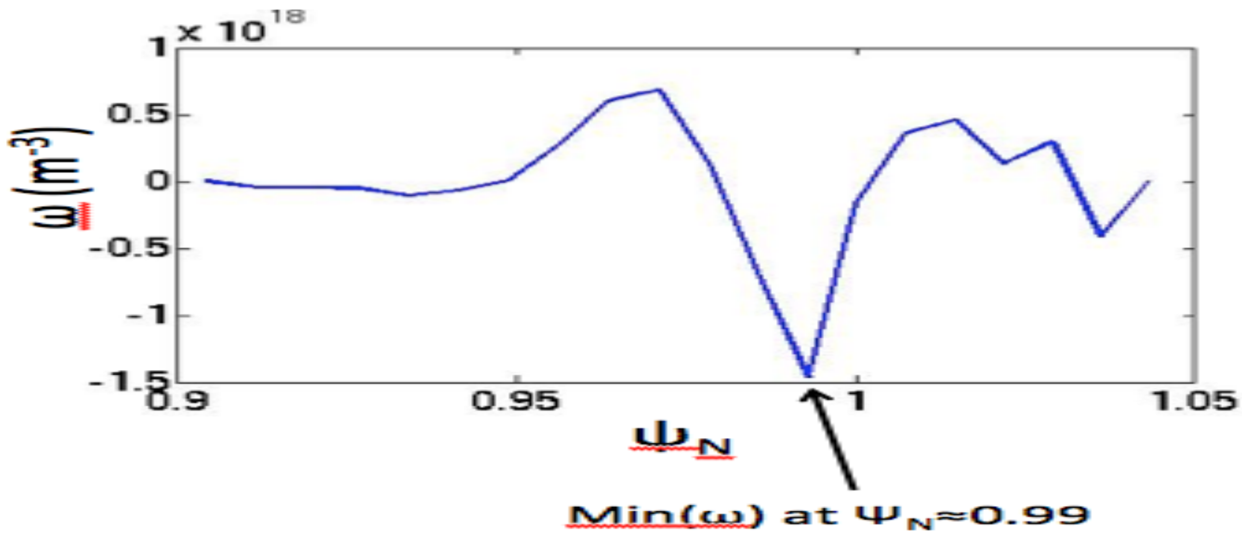




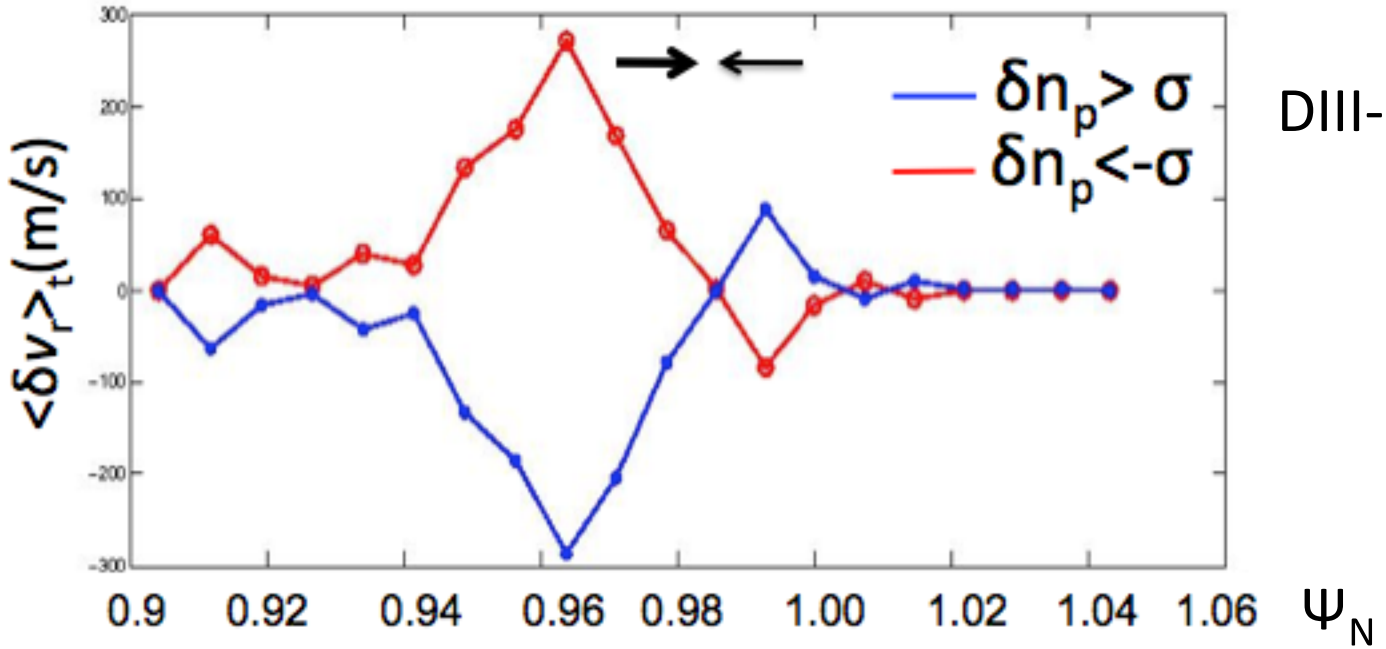
Vorticity merging

Vorticity merging with kinetic electrons, collisions and neutral recycling

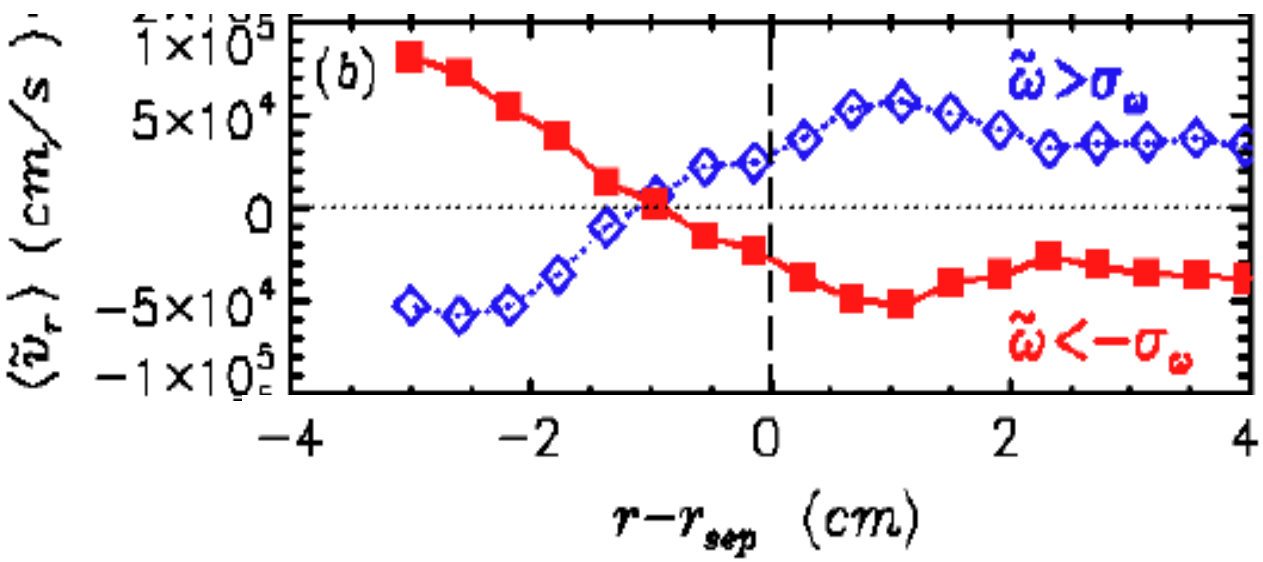




Apple-to-apple XGC1 & experiment comparision is needed



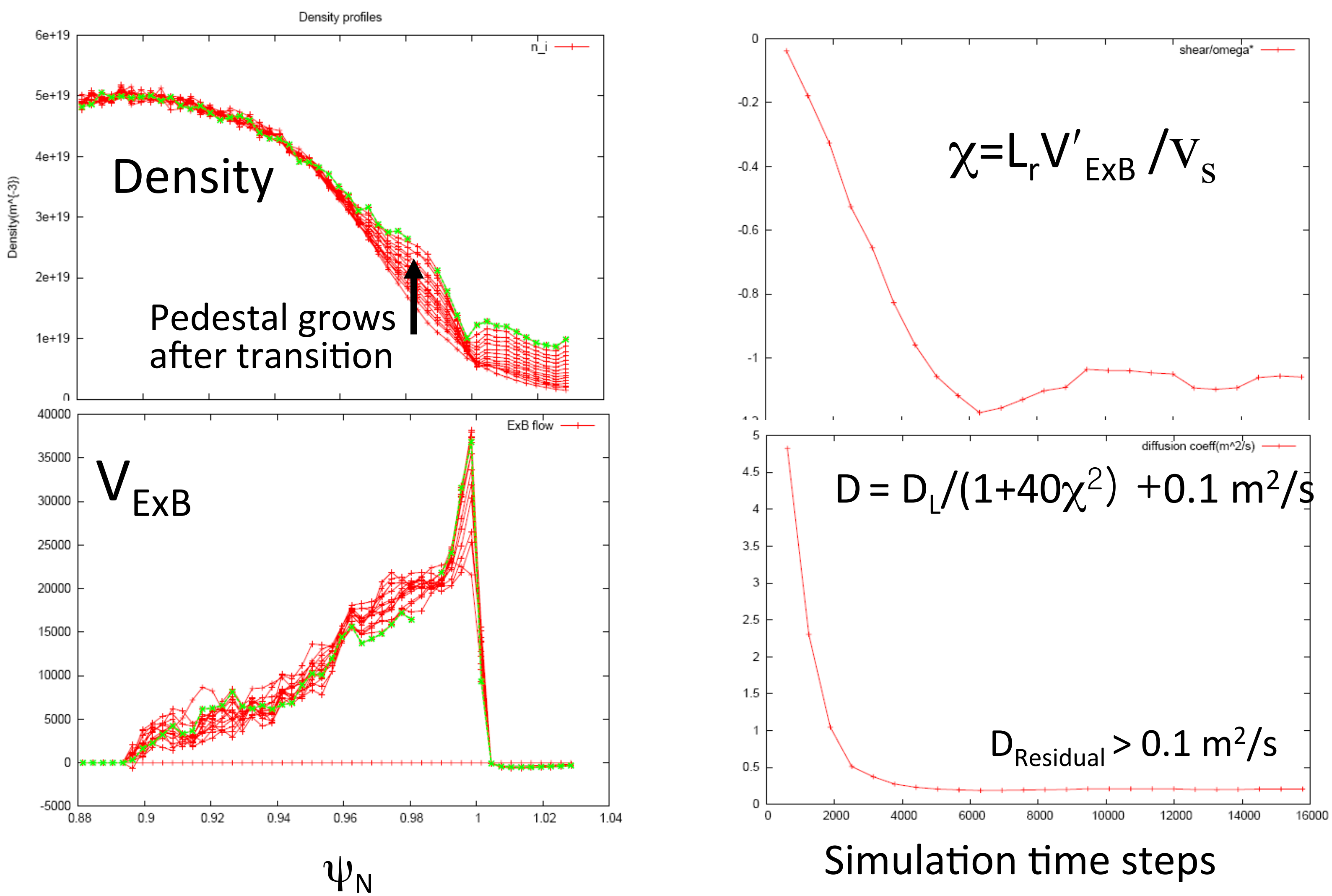
DIII-D



HL-2A

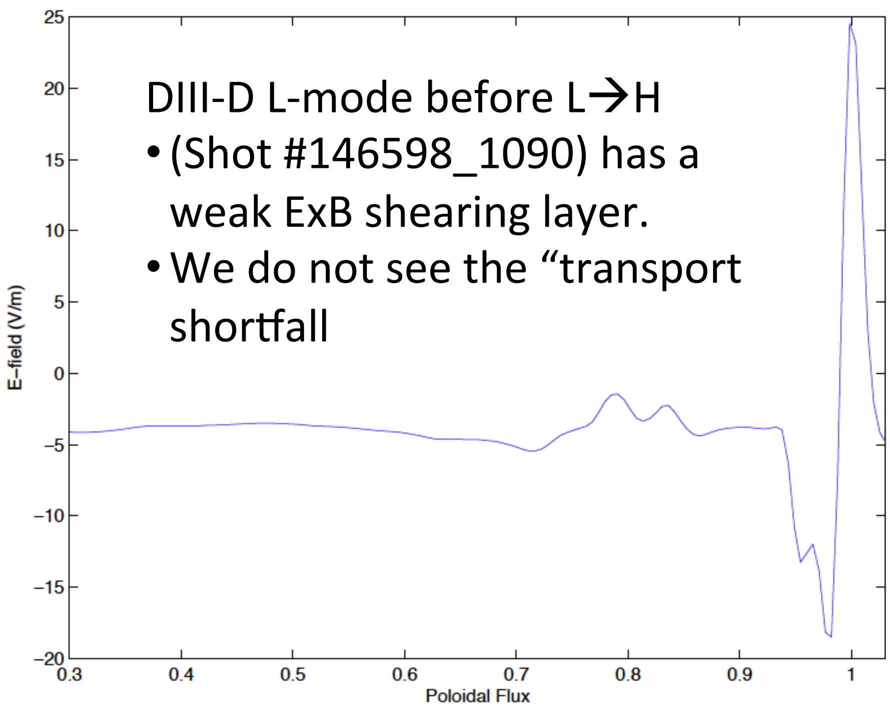
Nonlinear L-H transition from a conventional D(shear-suppression) model, with self-consistent plasma dynamics

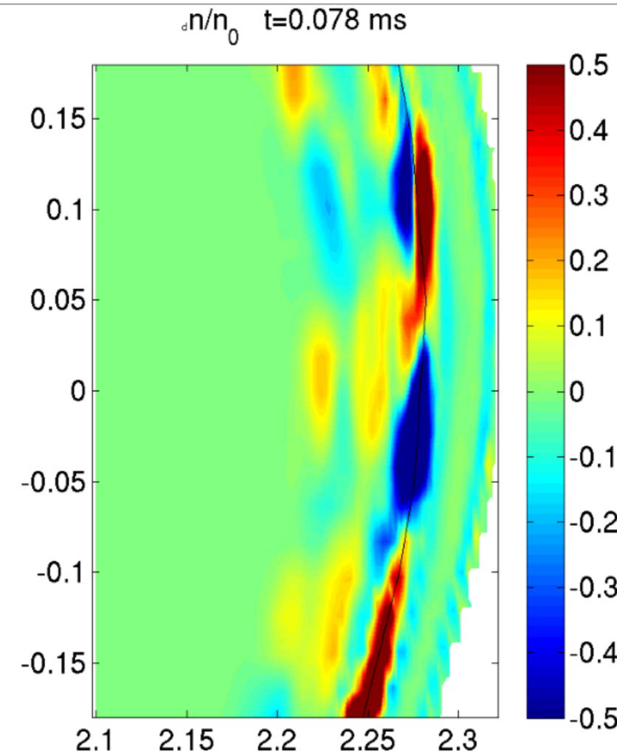
→ First-principles L-H transition in XGC1 will be tried in 2014



We have started the L-mode plasma simulation in route to L-H transition study in Boedo/McKee's DIII-D Plasma

- Nonlinear blobby turbulence, transport, role of collisions, roll of neutrals
  - Base case campaign is being done: without collisions or neutrals
  - Second campaign: with collisions and neutrals
  - Third campaign: continue the simulation to study the L-H transition at higher P_h
  - Fourth campaign: What happens after the L-H transition?



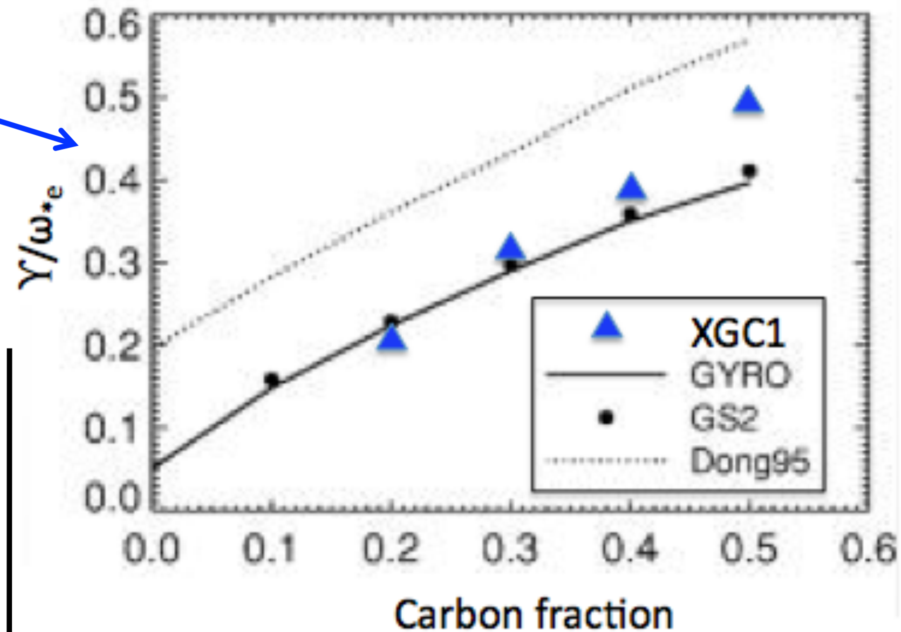


Outline

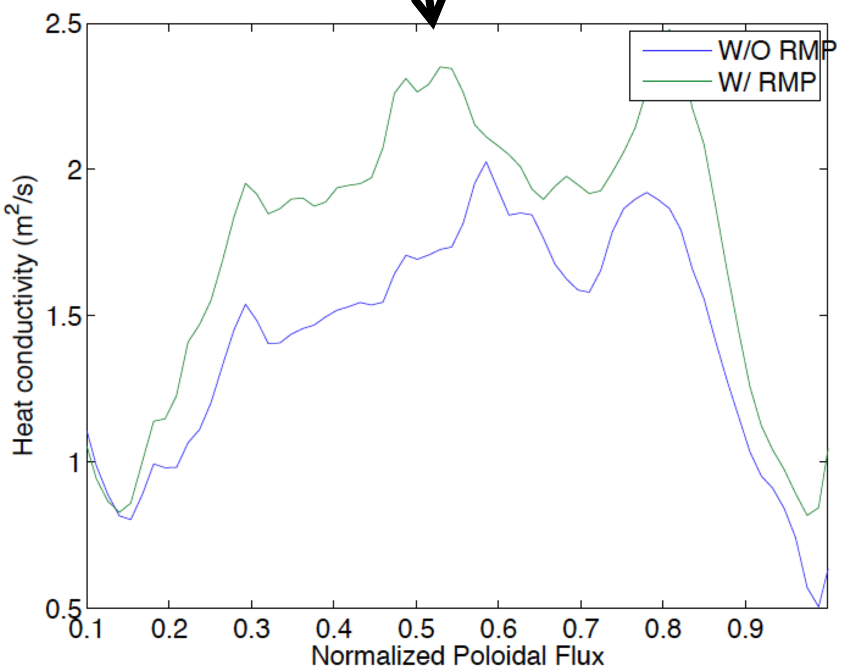
1) Brief introduction to XGC family codes
2) Present Capability of XGC1
    - Kinetic ion physics with MC neutral particles
    - New physics with kinetic electrons
    - Starting the quest for the L-H transition physics
3) Future Plans for XGC1
    - Impurity physics
    - L-H transition physics
    - E&M
    - Multiscale time integration between XGC1 and XGCa
    - 3D RMP penetration and transport
4) Summary

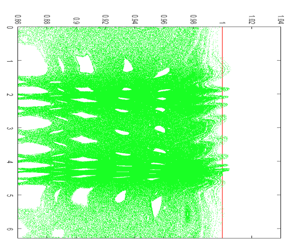
Upcoming new capabilities in XGC1

- Upcoming capabilities
  - Multiple impurity species
    - Collisional physics being verified
  - Electromagnetic turbulence
  - Turbulence in 3D magnetic perturbation (preliminary)



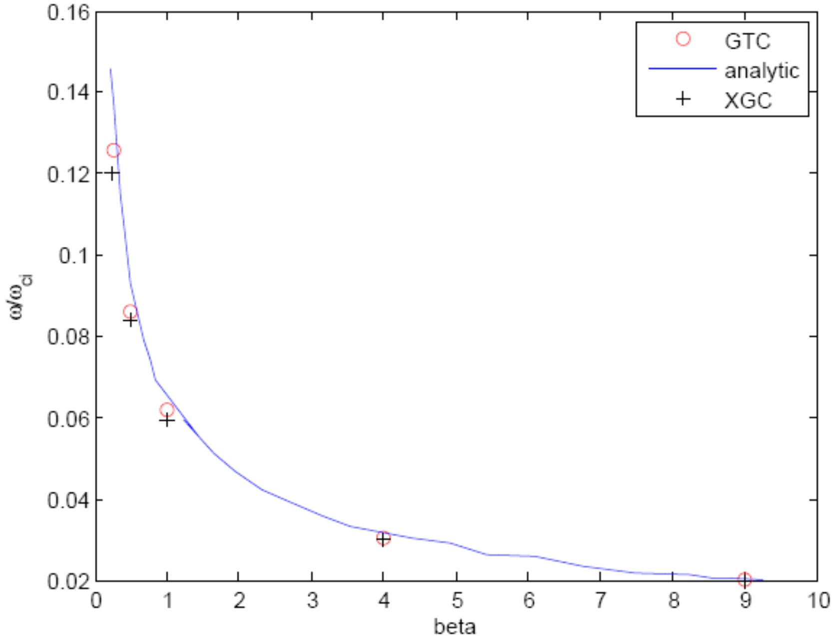
Collisionless Cross-verification of XGC1 Impurity Modes with GYRO and GS2 (K. Kim, KAIST).



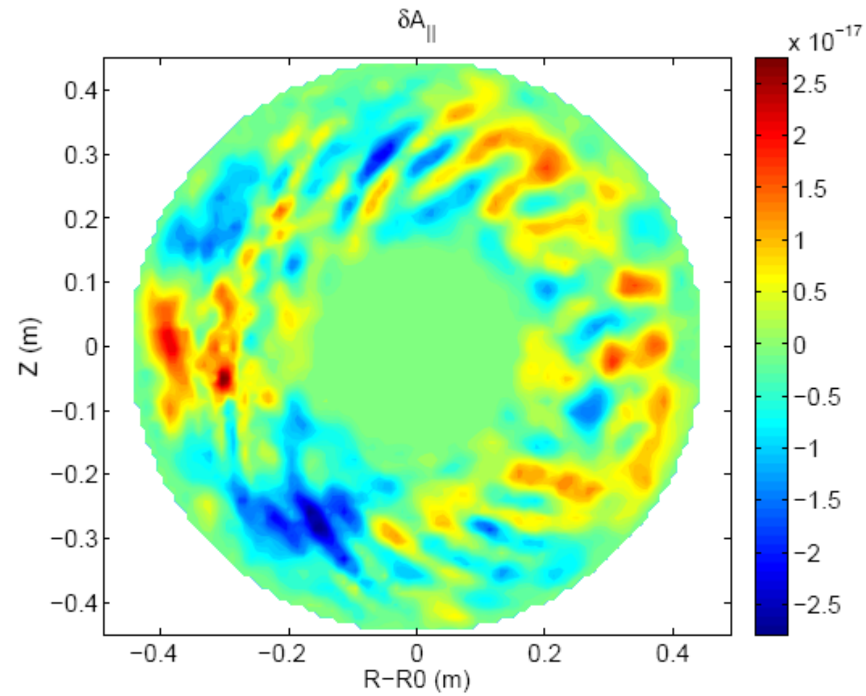


RMP-penetration solution imported from XGC0

We are moving the E&M turbulence capability to edge



Cross verification of Alfven wave frequency in XGC1 using **hybrid-electron** scheme (Collaboration with UC Irvine)



Low beta ITG turbulence from XGC1 using electromagnetic **split-weight** scheme (collaboration with U. Colorado)

- By this summer: GK ions + fluid electrons with kinetic electron closure [Chen11]
  - Include tearing parity modes (Lang-Ku, in collaboration with U. Colorado)
- E&M solver is being extended from reduced MHD to full MHD
- (Double) split-weight and hybrid electron schemes are also to be implemented

Continuity Eq. : The same except high order terms

GTC
$$\frac{\partial \delta n_e}{\partial t} + B_0 \mathbf{b}_0 \cdot \nabla\left(\frac{n_0 \delta u_{\parallel e}}{B_0}\right) + B_0 \mathbf{v}_E \cdot \nabla\left(\frac{n_0}{B_0}\right) - n_0(\mathbf{v}_* + \mathbf{v}_E) \cdot \frac{\nabla B_0}{B_0} = 0$$

GEM
$$\frac{\partial \delta n_e}{\partial t} + (B\nabla_\parallel + \delta \mathbf{B}_\perp \cdot \nabla)\frac{n_e u_{\parallel e}}{B} + \mathbf{v}_E \cdot \nabla n_e + \frac{1}{m_e \Omega_e B^2}\mathbf{B} \times \nabla B \cdot \nabla(\delta p_{\perp e} + \delta p_{\parallel e}) + \frac{2n_0}{B^3}\mathbf{B} \times \nabla B \cdot \nabla \phi = 0,$$

Ampere's Eq. & Vector potential: The same

$$n_0 e\, \delta u_{\parallel e} = \frac{c}{4\pi}\nabla_\perp^2 \delta A_\parallel + n_0 Z_i \delta u_{\parallel i} \qquad \delta E_\parallel = -\mathbf{b}_0 \cdot \nabla \delta\phi - \frac{1}{c}\frac{\partial \delta A_\parallel}{\partial t}$$

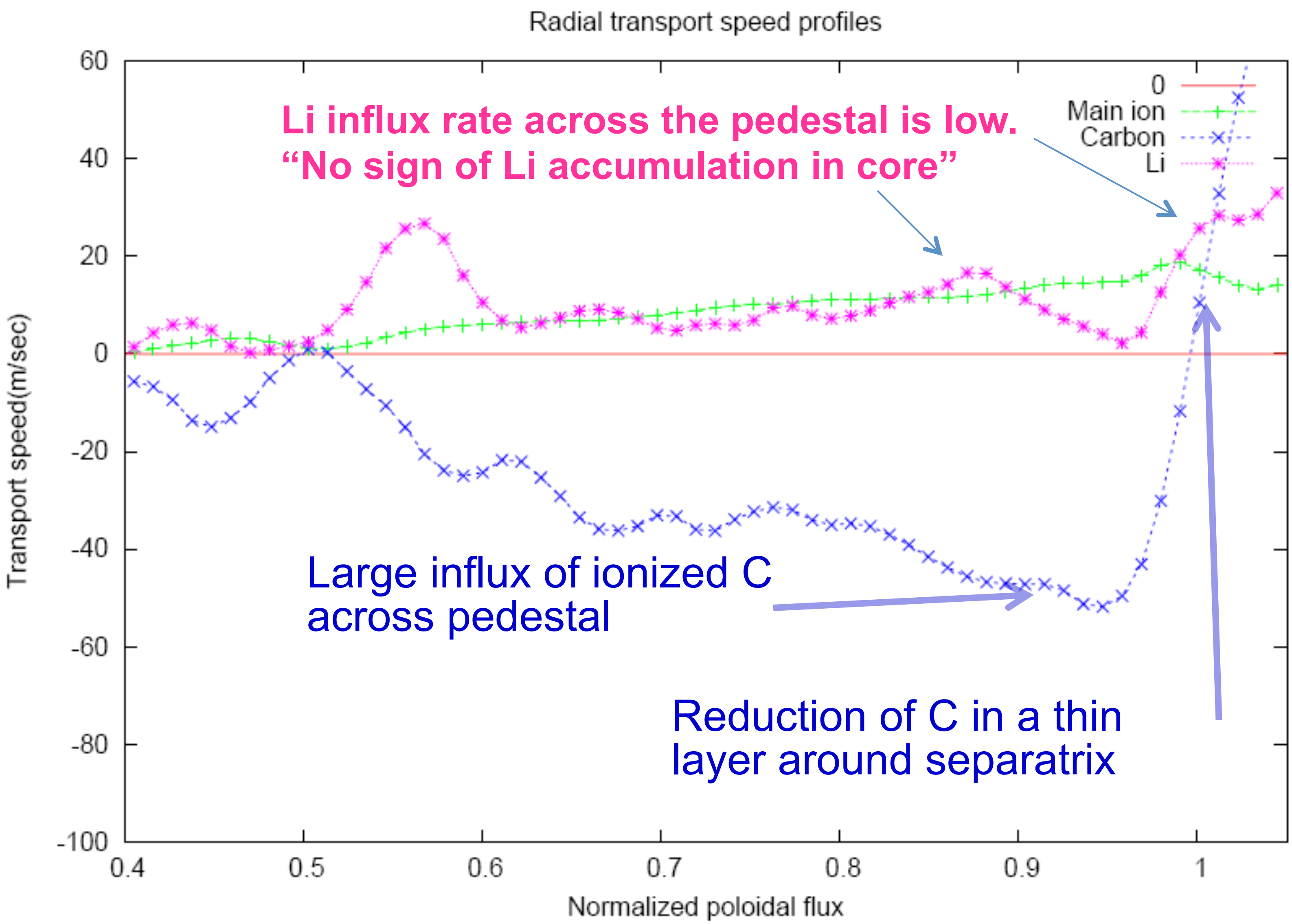
Ohm's Law:

GTC
$$\delta E_\parallel = -\mathbf{b}_0 \cdot \nabla \phi_{\mathrm{eff}}. \qquad \frac{e\phi_{\mathrm{eff}}^{(0)}}{T_e} = \frac{\delta n_e}{n_0} - \frac{\delta\psi}{n_0}\frac{\partial n_0}{\partial \psi_0} - \frac{\delta\alpha}{n_0}\frac{\partial n_0}{\partial \alpha_0}.$$
Details in next page

GEM
$$e n_0 E_\parallel = -\frac{\delta \mathbf{B}_\perp}{B} \cdot \nabla p_{\parallel 0} - b \cdot \nabla \delta p_\parallel + \eta_\parallel j_\parallel,$$
Massless fluid with resistivity

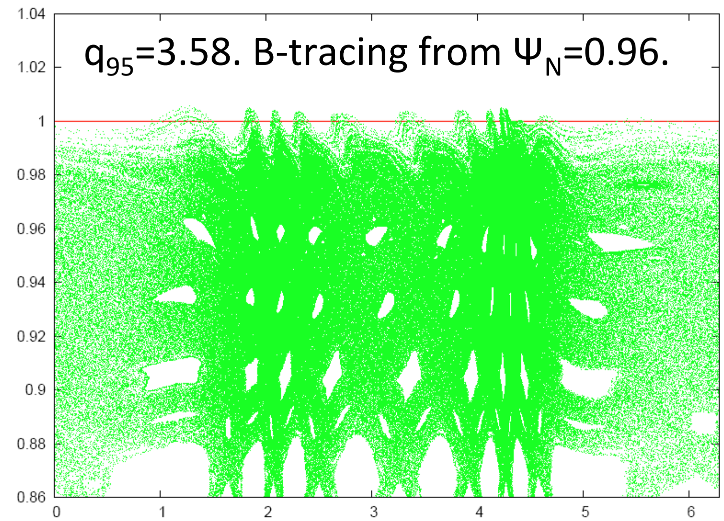
$$e n_0 E_\parallel - \frac{m_e}{\mu_0 e}(\nabla_\parallel \nabla_\perp^2 \phi + \nabla_\perp^2 E_\parallel) = -\nabla \cdot \int m_e v_\parallel v_G f_{e1} dv - \int \mu b \cdot \nabla B_0 f_{e1} dv + \text{ion terms},$$
Kinetic closure

Neoclassical XGC0 says, at n_C/n_e=10%, Li moves outward while C^{+6} moves inward at ψ_N<1.



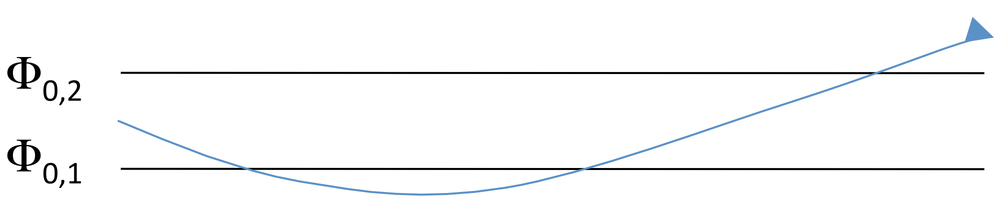
RMP Penetration & Plasma Transport in XGC0

- Realistic Diverted geometry:EFIT
- Magnetic equilibrium and perturbation solver from M3D: $\delta\psi(\delta J_T)$
- Monte Carlo neutral particles with wall-recycling
- Experimental level of heat and momentum source at core-edge boundary
- Random-walk modeling of anomalous transport to reproduce pre-RMP plasma



Assumptions for the RMP study in XGC0

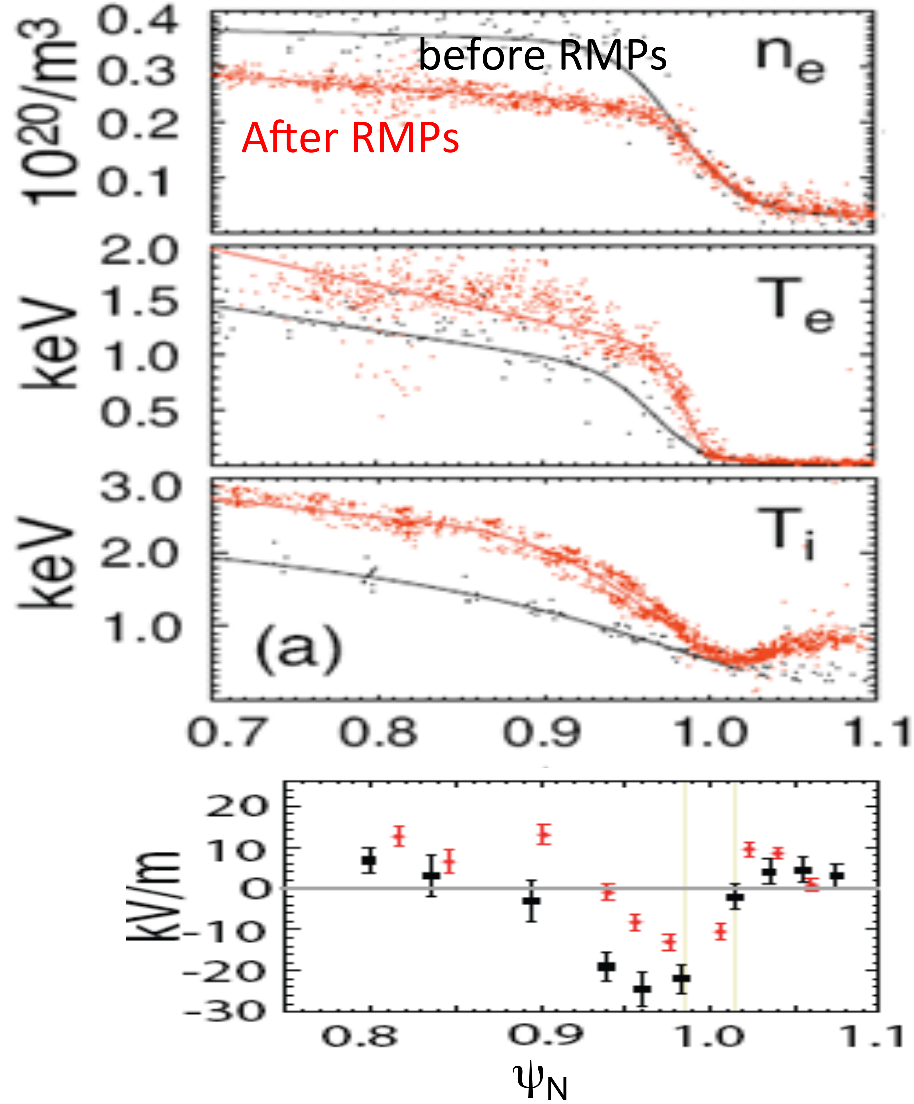
- Small 3D $\delta B \ll B_0$
- $\nabla p(\psi_0)$ are supported by partial stochasticity and the ψ_0-aligned cantori
  → $\nabla\Phi(\psi_0)$ holds, $E_{||}$ is from $b\cdot\nabla_\psi\Phi$
- Qusi-steady solution exist $\partial A_{||}/\partial(t/\tau_{Alfven}) \rightarrow 0$, $(\mathbf{E}_{||} = -\delta b_r \nabla_r \Phi(r) - \partial \mathbf{A}_{||}/\partial t)$
- Assume that turbulence-driven transport is small compared to RMP-driven transport



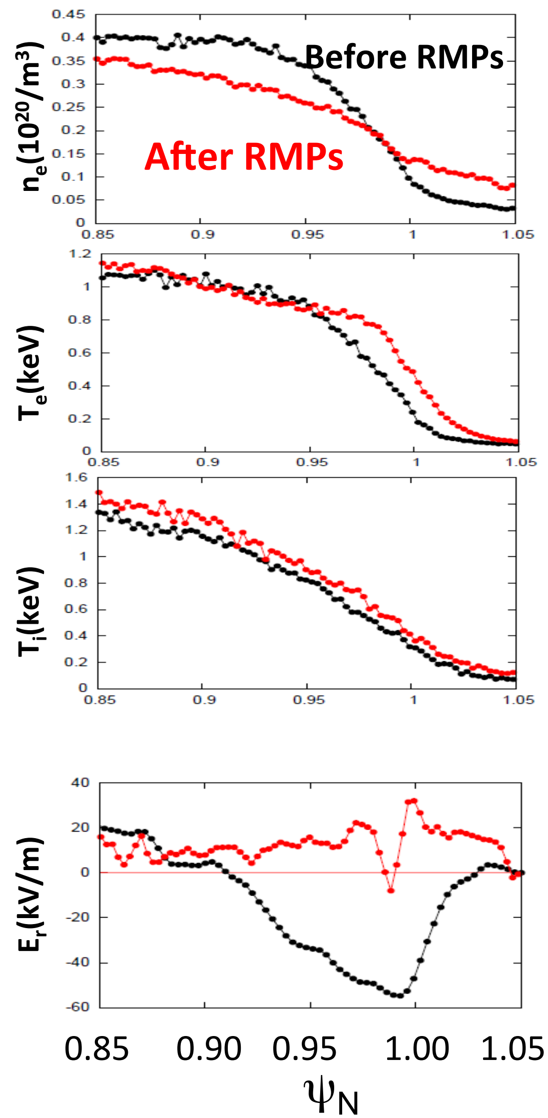
$B=B_0+\delta B$

$E_{||}= -\nabla\Phi_0 \bullet \delta B_r/B_0$

Simulation reproduces all the qualitative features of experiment, inside the ELM suppression window (q_{95}=3.58)



DIII-D Experiment 126006 at ~100 ms after RMPs



Density pump-out

Te shifted radially or steepens

Er shearing rate survives

Simulation. at 4ms after the RMP turn-on: still evolving.

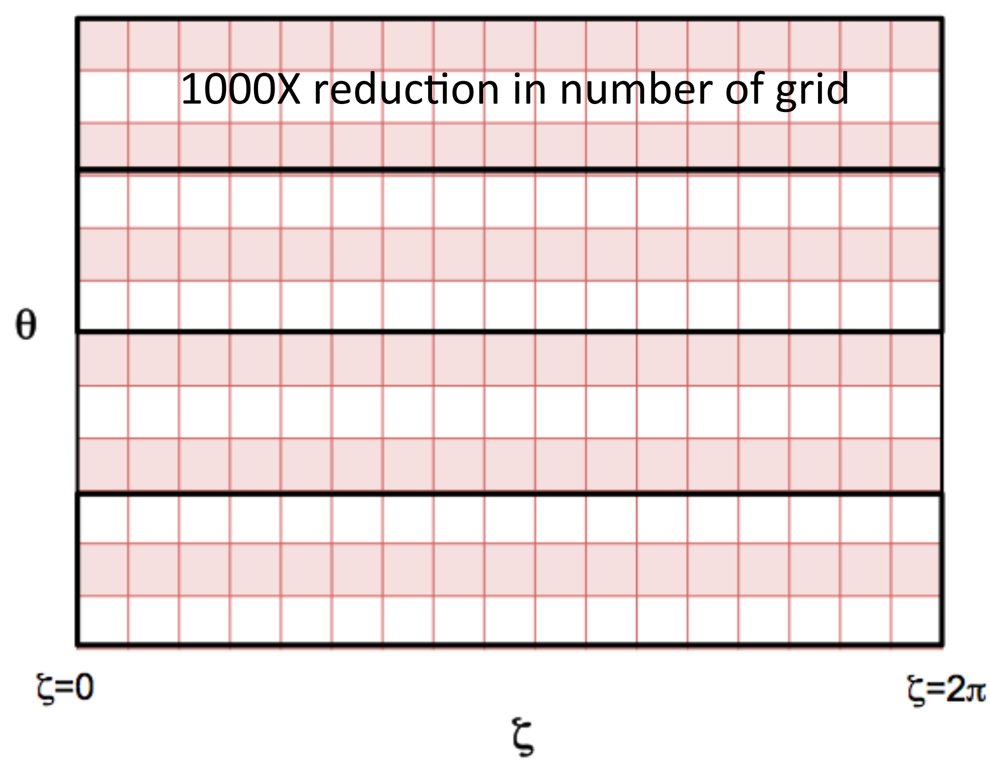
An Example Challenge in EPSI, requiring collaboration with all four Institutes+

Multi-scale Time Advancement

- Prolong the high fidelity simulation to experimental edge transport time scale
- Time consuming turbulence simulation may not be needed at all time steps
- Divide XGC1 in XGC^F(axisymmetric+turbulence) and XGC^C(axisymmetric)
- Use the Φ^F(turbulence) data in XGC^C, with updates as needed

- Perform the computation of XGC^C and XGC^F at data source.
- Minimal loss of kinetic information in restricting and lifting.
  - Common (gyrokinetic)equations between fine and coarse grained systems

Grid coarsening and refining for restricting and lifting

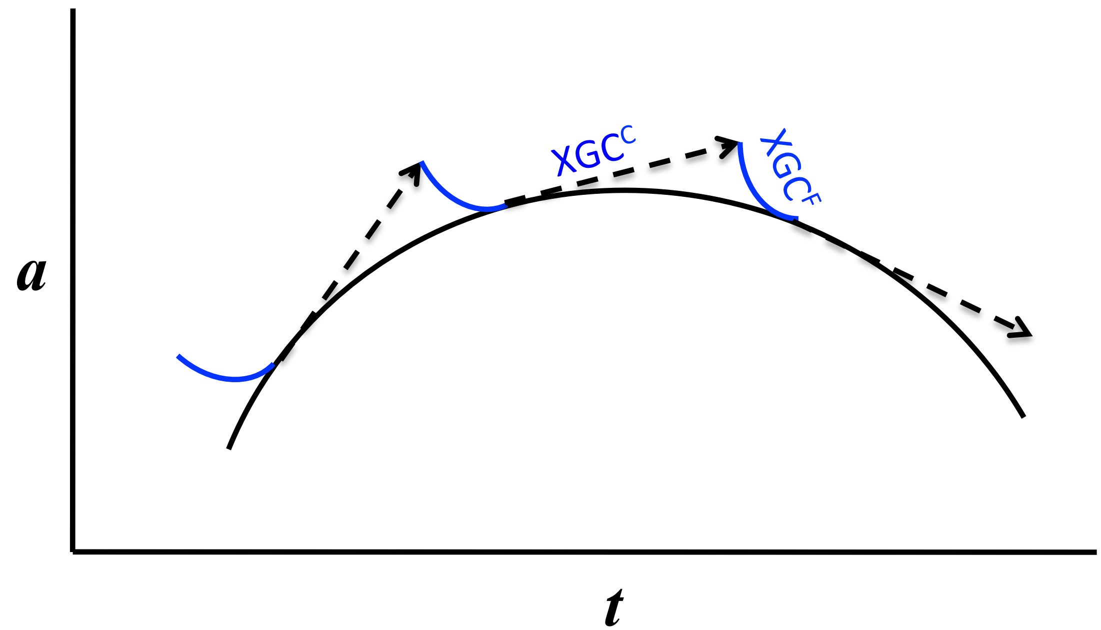


Questions to study

- Time steps ΔT^C and ΔT^F?
- Stability?
- Stiff profile?
- Solution bifurcation?

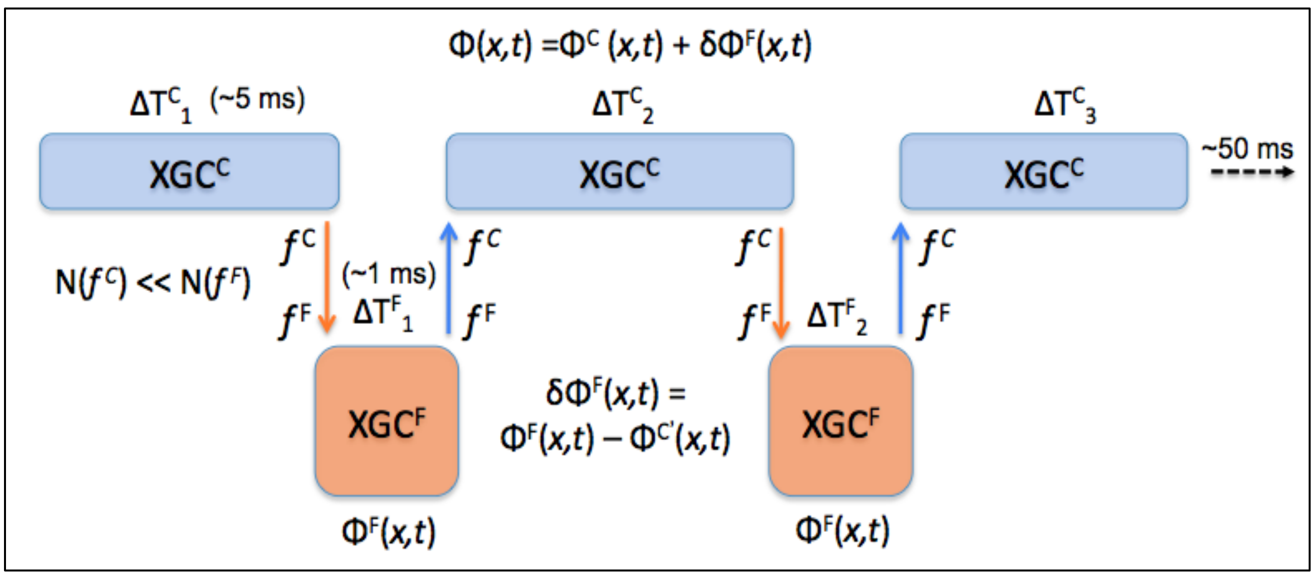
→Heavy usage of data management, math and analysis in-memory.

Collaboration with SUPER and QUEST is essential



$G^F(d; f^F, D) = 0$
$G^C(d, D; f^C) = 0$

- d=B.D. condition, heating profile, etc.
- $D = \Phi^F(x,t)$
- Tighter than the Heterogeneous Multiscale Method



Summary

- Present version XGC1 simulates a comprehensive electrostatic edge transport physics in diverted geometry (pedestal+SOL+core): including kinetic ion+electron turbulence, neoclassical, neutral recycling, nonlinear collisions, impurity radiation, and logical sheath.
- XGC1 simulates edge blobs
- Measures heatload footprint on realistic-geometry divertor plates.
- Calculates the intrinsic edge momentum source and its inward transport
- XGC1 started the quest for the L-H transition physics
  - Verified correlation of $P_{L\text{-}H}$ with neoclassical ExB shearing rate.
  - Finds vorticity merging in pedestal (strengthening the mean ExB shearing rate).
  - L-H transition is to be attempted in 2014
- XGC1 is presently electromagnetic in the core delta-f plasma: The E&M capability is currently being move to diverted edge (Lang, Ku, Chen).
- Multiacle XGC1-XGCa framework is being developed in EPSI
- RMP physics capability is to be moved from XGC0 to XGC1 (Hager)